

10/074,895

=> file casreact

FILE 'CASREACT' ENTERED AT 15:37:05 ON 25 JAN 2005

USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 23 Jan 2005 VOL 142 ISS 4

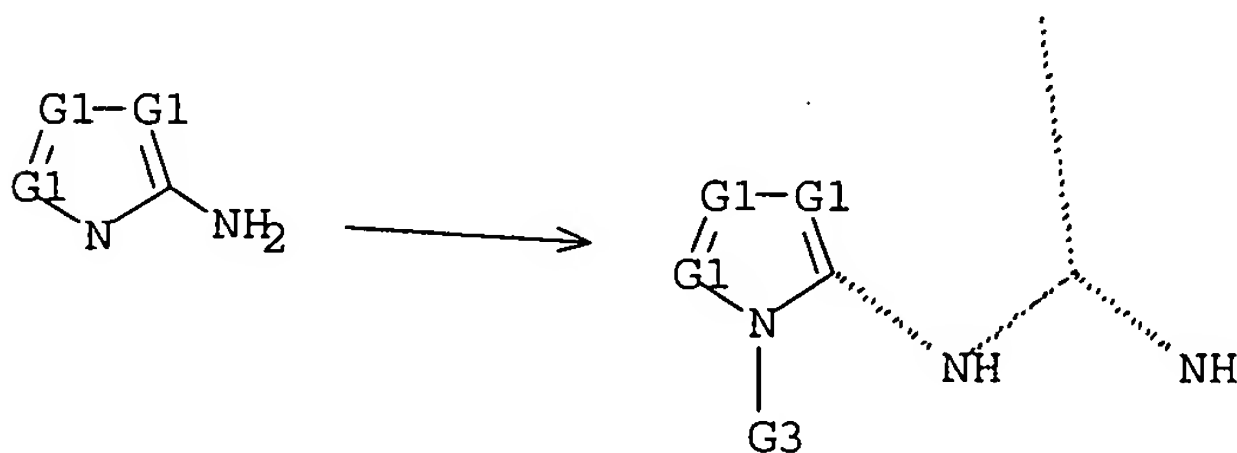
\*\*\*\*\*  
\*  
\* CASREACT now has more than 8 million reactions \*  
\*  
\*\*\*\*\*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d que

L1 STR



G1 C,N

G2 O,S

G3 Cb,Cy,Hy

Structure attributes must be viewed using STN Express query preparation.

L3 24 SEA FILE=CASREACT SSS FUL L1 ( 189 REACTIONS)

=> d l3 1-24 ibib abs fcrd

L3 ANSWER 1 OF 24 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 141:395467 CASREACT

TITLE: 3-(p-Bromophenyl)-5-aminopyrazole and some derivatives

AUTHOR(S): Nam, N. L.; Grandberg, I. I.; Sorokin, V. I.

CORPORATE SOURCE: Kafedra Org. Khim., Timiryazevsk. S-Kh. Akad., Russia

SOURCE: Izvestiya Timiryazevskoi Sel'skokhozyaistvennoi

Akademii (2003), (4), 142-146

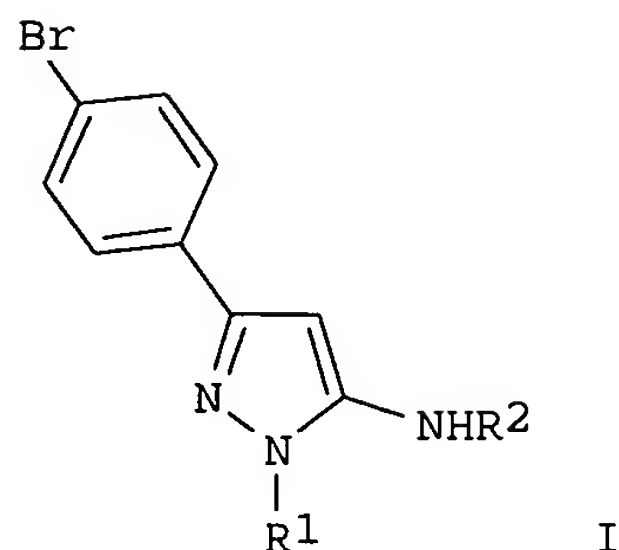
CODEN: ITSAA7; ISSN: 0021-342X

PUBLISHER: ANO "Izdatel'stvo MSKhA"

DOCUMENT TYPE: Journal

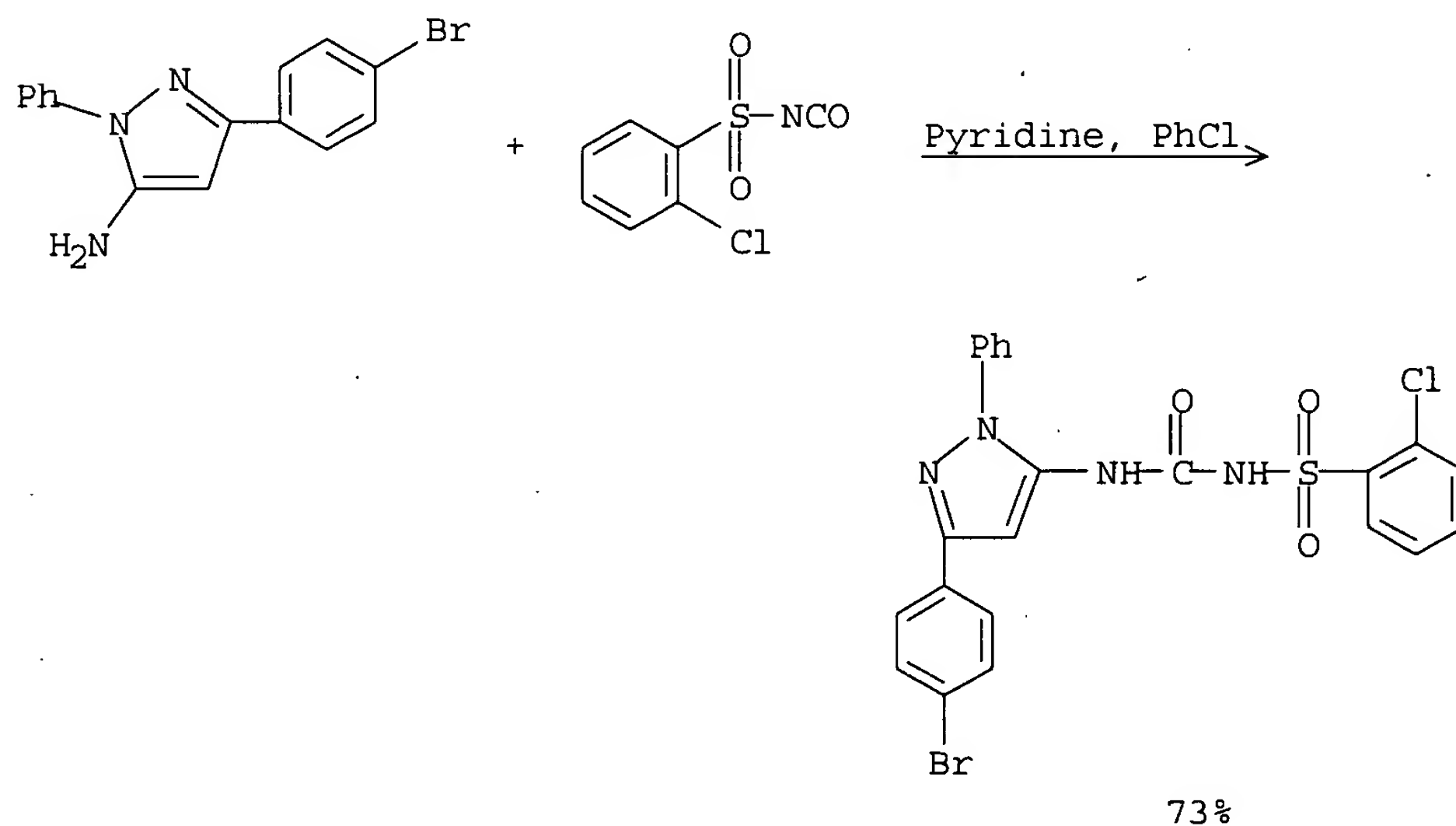
LANGUAGE: Russian

GI



AB 5-Aminopyrazoles I (R1 = H, Me, Ph; R2 = H) were readily prepared via cyanation of  $\alpha$ ,4-dibromoacetophenone with sodium cyanide followed by heterocyclization of 4-bromo- $\alpha$ -cyanoacetophenone with the corresponding hydrazines. Pyrazole I (R1 = Ph; R2 = H) was further functionalized by reactions with acyl and sulfonyl halides, anhydrides or isocyanates to give I (R1 = Ph; R2 = MeCO, PhCO, 4-MeC6H4SO2, 2-ClC6H4SO2NHCO).

RX(5) OF 19



L3 ANSWER 2 OF 24 CASREACT COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 140:59611 CASREACT  
 TITLE: Chemistry of Substituted Quinolinones. Part 8.  
 Synthesis and Cyclization Reactions of Ethyl  
 5-Amino-1-(1-methyl-2-oxoquinolin-4-yl)-3-  
 methylsulfonylpyrazole-4-carboxylate  
 AUTHOR(S): Abass, Mohamed  
 CORPORATE SOURCE: Ain Shams University, Cairo, Egypt  
 SOURCE: Phosphorus, Sulfur and Silicon and the Related  
 Elements (2003), 178(7), 1413-1432  
 CODEN: PSSLEC; ISSN: 1042-6507  
 PUBLISHER: Taylor & Francis, Inc.

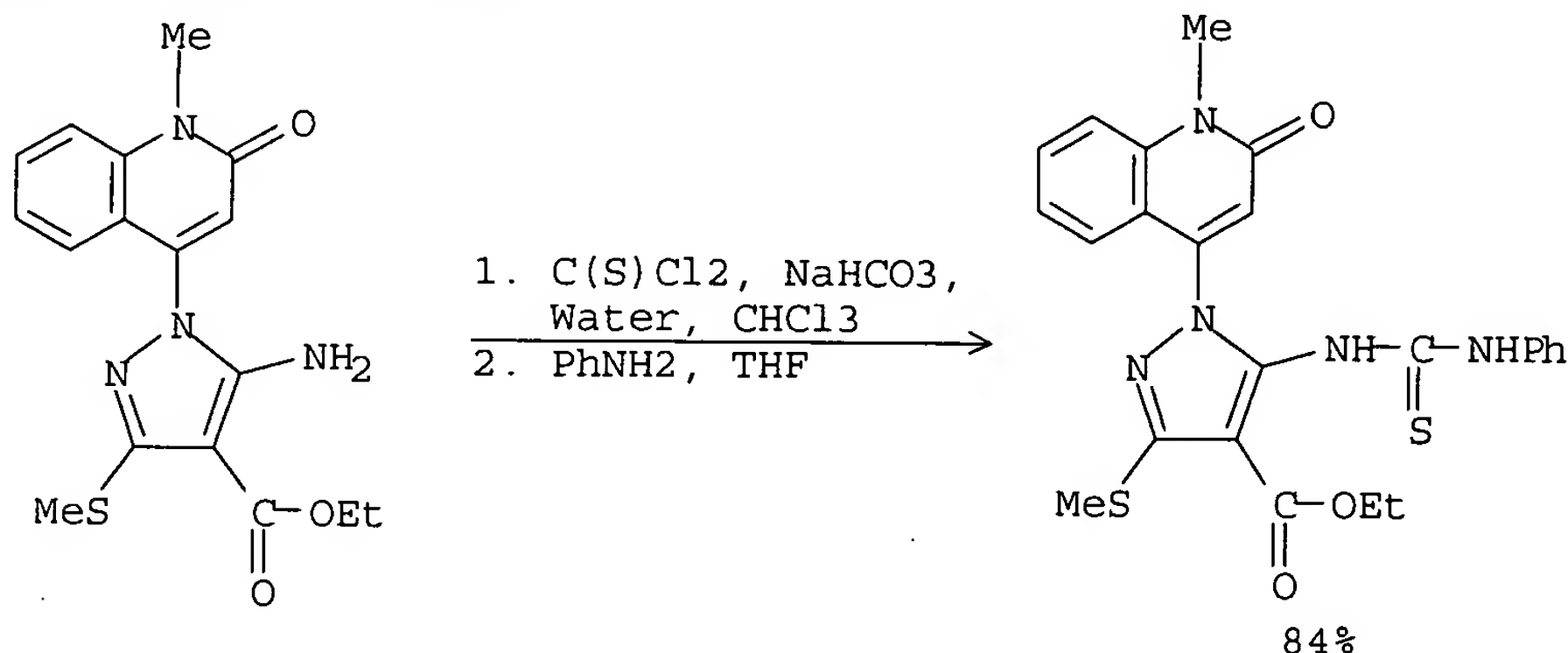
10/074,895

DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The synthesis of the titled amino-ester I [R1 = Et; R2 = NH2(II)] is described and its hydrolysis and chloroacetylation led to the acid I (R1 = H; R2 = NH2) and acetamide I (R1 = Et; R2 = NHCOCH2Cl), which were cyclized to the pyrazolopyridones III (R = H) and III (R = Cl), resp. Condensation of II with 2,5-dimethoxytetrahydrofuran afforded the pyrrolylpyrazole I (R1 = Et; R2 = pyrrolo), which underwent cyclization by action of PPA to give pyrazolopyrrolizine IV. Treating II with thiophosgene gave the pyrazolyl isothiocyanate I (R1 = Et; R2 = NCS), which added aniline to yield the thiourea derivative I (R1 = Et; R2 = NHCSNHPh), and cyclized to give pyrazolopyrimidinethiones V (R = H, NH2, Ph). Condensation of II with formamide furnished pyrazolopyrimidine VI (R = H), while with tri-Et orthoformate produced the ethoxymethyleneaminopyrazole I (R1 = Et; R2 = N:CHOEt), which condensed with hydrazine to give the aminopyrazolopyrimidine VI (R = NH2). Reaction of II with Lawesson's reagent resulted in the pyrazolothiazaphosphinine VII. Also the cyclization reaction of the compound II with malononitrile and its mixts. with carbon disulfide, Ph isothiocyanate, or benzaldehyde led to the formation of a variety of polyfunctional substituted pyrazolopyrimidines, pyrazolothiazine and pyrazolopyridine.

RX(41) OF 56 - 2 STEPS



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 24 CASREACT COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 139:301299 CASREACT  
TITLE: Structure-Activity Relationships of the p38 $\alpha$  MAP  
Kinase Inhibitor 1-(5-tert-Butyl-2-p-tolyl-2H-pyrazol-3-yl)-3-[4-(2-morpholin-4-yl-ethoxy)naphthalen-1-yl]urea (BIRB 796)  
AUTHOR(S): Regan, John; Capolino, Alison; Cirillo, Pier F.;  
Gilmore, Thomas; Graham, Anne G.; Hickey, Eugene;  
Kroe, Rachel R.; Madwed, Jeffrey; Moriak, Monica;  
Nelson, Richard; Pargellis, Christopher A.; Swinamer,

10/074,895

CORPORATE SOURCE: Alan; Torcellini, Carol; Tsang, Michele; Moss, Neil  
Department of Medicinal Chemistry, Boehringer  
Ingelheim Pharmaceuticals Research and Development  
Center, Ridgefield, CT, 06877, USA  
SOURCE: Journal of Medicinal Chemistry (2003), 46(22),  
4676-4686  
CODEN: JMCMAR; ISSN: 0022-2623  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB We report on the structure-activity relationships (SAR) of  
1-(5-tert-butyl-2-p-tolyl-2H-pyrazol-3-yl)-3-[4-(2-morpholin-4-yl-  
ethoxy)naphthalen-1-yl]urea (BIRB 796), an inhibitor of p38 $\alpha$  MAP  
kinase which has advanced into human clin. trials for the treatment of  
autoimmune diseases. Thermal denaturation was used to establish mol.  
binding affinities for this class of p38 $\alpha$  inhibitors. The tert-Bu  
group remains a critical binding element by occupying a lipophilic domain in  
the kinase which is exposed upon rearrangement of the activation loop. An  
aromatic ring attached to N-2 of the pyrazole nucleus provides important  
 $\pi$ -CH<sub>2</sub> interactions with the kinase. The role of groups attached  
through an ethoxy group to the 4-position of the naphthalene and directed  
into the ATP-binding domain is elucidated. Pharmacophores with good  
hydrogen bonding potential, such as morpholine, pyridine, and imidazole,  
shift the melting temperature of p38 $\alpha$  by 16-17° translating into K<sub>d</sub>  
values of 50-100 pM. Finally, we describe several compds. that potently  
inhibit TNF- $\alpha$  production when dosed orally in mice.

RX(4) OF 120 - REACTION DIAGRAM NOT AVAILABLE

REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 24 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 139:85341 CASREACT  
TITLE: Method for preparation of new N-substituted  
derivatives of 5-amino-1-phenylpyrazole, the  
derivatives, and their use as parasitocidal and/or  
insecticidal agents  
INVENTOR(S): Bertrand, Guy; Romanenko, Vadim D.; Raynier, Bernard;  
Derrieu, Guy  
PATENT ASSIGNEE(S): Virbac SA, Fr.  
SOURCE: Fr. Demande, 87 pp.  
CODEN: FRXXBL  
DOCUMENT TYPE: Patent  
LANGUAGE: French  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

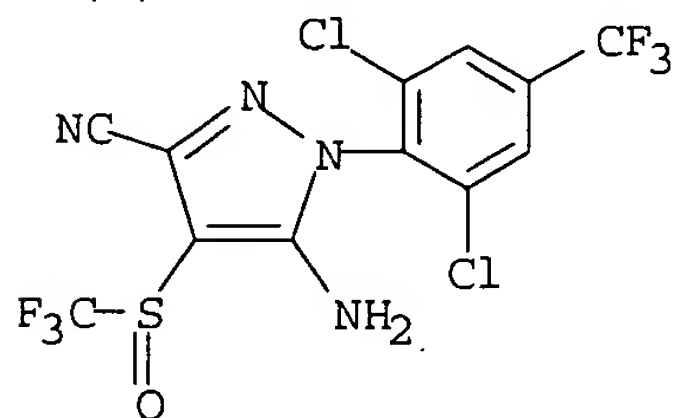
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2834288	A1	20030704	FR 2001-17018	20011228
PRIORITY APPLN. INFO.:			FR 2001-17018	20011228
OTHER SOURCE(S):	MARPAT 139:85341			
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The invention provides new derivs. of 5-amino-1-phenylpyrazoles,  
specifically I [wherein: A, B = H, (a)cyclic alk(en/yn)yl (optionally

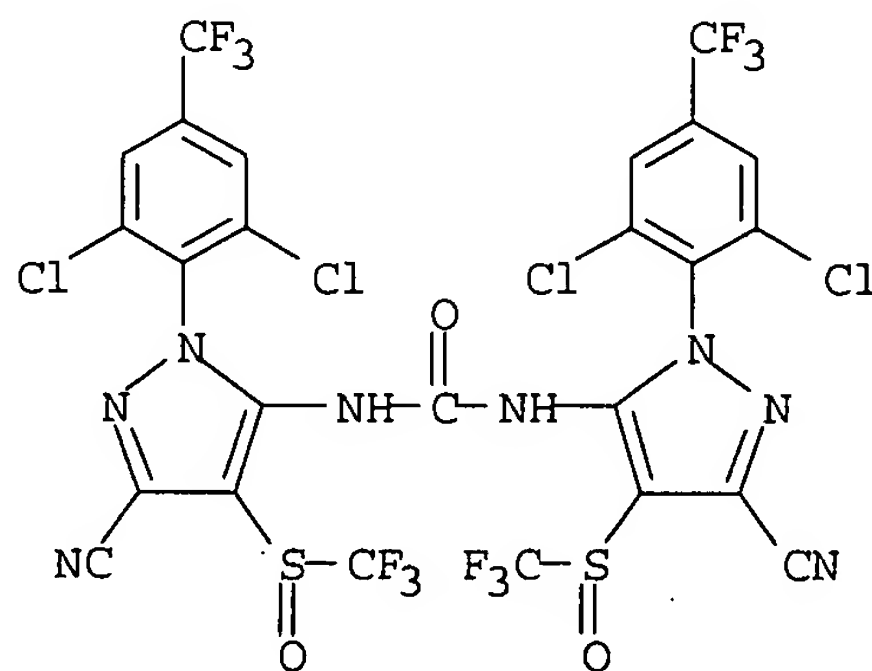
substituted by one or more halo, alkoxy, alkylthio, or alkoxycarbonyl), halo, cyano, thiocyno, nitro, sulfamido, (di)alkylamino, aminocarbonyl, aminothiocarbonyl, (di)alkylaminocarbonyl, (di)alkylaminothiocarbonyl, alkylcarbonylamino, alkylthiocarbonylamino, S(O)nR [n = 0, 1, or 2, and R = (a)cyclic, (un)saturated (halo)alkyl], Ph, phenylalkyl, or 4- to 7-membered heterocyclyl with 1-3 N/O/S/Si atom(s); R1, R2, R3, R4, and R5 = H, halo, (a)cyclic (un)saturated C1-6 (halo)alkyl, (halo)alkoxy, or (halo)alkylthio; Z = -N:C:O, -N:C:S, -N:S:O, -NHC(:X)R6, -NHC(:O)XR6, -NHC(:S)XR6, -NHC(:X)NR7R8; X = O or S; R6 = (un)substituted (a)cyclic alk(en/yn)yl, Ph, phenylalkyl, or heterocyclyl; R7, R8 = H, groups given for R6, dimeric unit of I; also Z = -N:C:N- forming a dimer of I; or Z = (un)substituted 1,2-thiazin-2-yl 1-oxide motif]. The invention also comprises processes for preparation of I from corresponding amines I [Z = NH2], typically via reaction of the amines with phosgene, thiophosgene, or thionyl chloride, and optionally reaction of the resultant I [Z = isocyanato, isothiocyanato, or N-sulfinylamino (i.e., -N:S:O)]. Compds. I can be administered to vertebrates, particularly domesticated animals, either orally, topically, or parenterally. In general, I can be used to control both arthropods and nematodes which are parasites of both animals and plants, by application to either the hosts or their environments. Over 30 specific compds. were claimed per se. Examples (23) include synthesis, and both agrochem. and pharmaceutical formulations. For instance, the amine precursor II [Z = NH2] reacted with phosgene in anhydrous PhMe in the presence of 2 equiv pyridine to give II [Z = isocyanato] in 95% yield. Reaction of this isocyanate with 3,5-bis(trifluoromethyl)aniline gave title compound III. Compds. I were against the stablefly *Stomoxys calcitrans* in a Petri dish experiment, at dosages of 0.1 to 30 µg/fly. An exemplary injectable contained 1% I, 30% Et oleate, and sesame oil qsp 100%, and was sterilized by membrane filtration.

RX(9) OF 11



(step 1)

1. Pyridine, CH<sub>2</sub>Cl<sub>2</sub>, PhMe
2. COCl<sub>2</sub>, PhMe
3. CH<sub>2</sub>Cl<sub>2</sub>



92%

REFERENCE COUNT:

7

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/074,895

L3 ANSWER 5 OF 24 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 138:24709 CASREACT  
TITLE: Preparation of pyrazole compds. and bis  
pyrazole-1H-pyrazole intermediates as antiinflammatory  
agents  
INVENTOR(S): Kapadia, Suresh R.; Song, Jinhua J.; Yee, Nathan K.  
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA  
SOURCE: U.S., 37 pp., Cont.-in-part of U.S. 6,372,773.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 3  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6492529	B1	20021210	US 2002-67492	20020205
US 6319921	B1	20011120	US 2000-484638	20000118
US 6333325	B1	20011225	US 2001-871559	20010531
US 6329415	B1	20011211	US 2001-891579	20010626
US 2002065285	A1	20020530	US 2001-891820	20010626
US 6506748	B2	20030114		
US 6372773	B1	20020416	US 2001-920899	20010802
PRIORITY APPLN. INFO.:			US 2000-484638	20000118
			US 2001-920899	20010802
			US 1999-116400P	19990119
			US 2001-891579	20010626

OTHER SOURCE(S): MARPAT 138:24709  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Pyrazole compds., e.g. I, as well as bis pyrazole-1H-pyrazole intermediate compds. e.g. II, were prepared The compds. are useful in pharmaceutic compns. for treating diseases or pathol. conditions involving inflammation such as chronic inflammatory diseases. All prepared compds. had IC50 < 10 mM for inhibition of TNF $\alpha$  in lipopolysaccharide stimulated THP cells.

RX(1) OF 282 - REACTION DIAGRAM NOT AVAILABLE

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 24 CASREACT COPYRIGHT 2005 ACS on STN

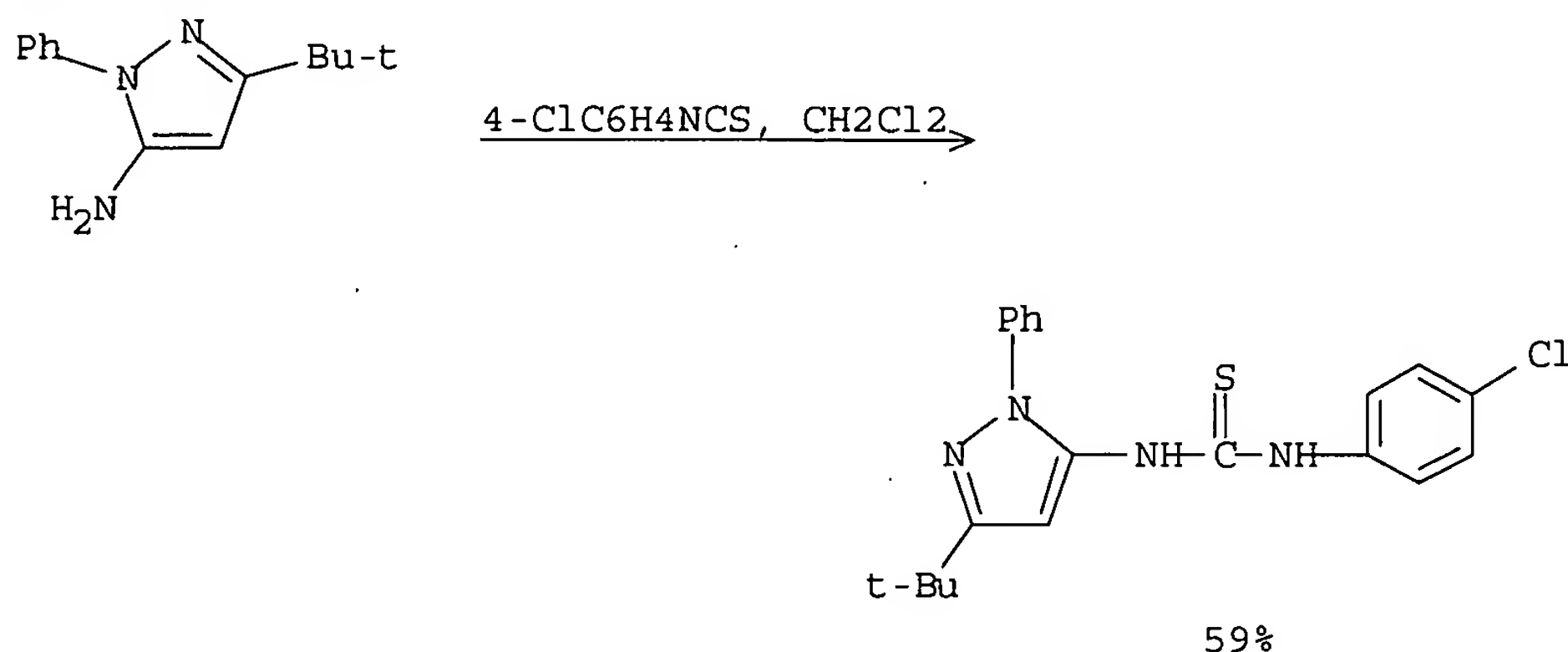
ACCESSION NUMBER: 137:119059 CASREACT  
TITLE: Pyrazole Urea-Based Inhibitors of p38 MAP Kinase: From Lead Compound to Clinical Candidate  
AUTHOR(S): Regan, John; Breitfelder, Steffen; Cirillo, Pier; Gilmore, Thomas; Graham, Anne G.; Hickey, Eugene; Klaus, Bernhard; Madwed, Jeffrey; Móriak, Monica; Moss, Neil; Pargellis, Chris; Pav, Sue; Proto, Alfred; Swinamer, Alan; Tong, Liang; Torcellini, Carol  
CORPORATE SOURCE: Research and Development Center, Department of Medicinal Chemistry, Boehringer Ingelheim Pharmaceuticals, Ridgefield, CT, 06877, USA  
SOURCE: Journal of Medicinal Chemistry (2002), 45(14), 2994-3008  
CODEN: JMCMAR; ISSN: 0022-2623

10/074,895

PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB We report on a series of N-pyrazole, N'-aryl ureas and their mode of binding to p38 mitogen activated protein kinase. Importantly, a key binding domain that is distinct from the ATP (ATP) binding site is exposed when the conserved activation loop, consisting in part of Asp168-Phe169-Gly170, adopts a conformation permitting lipophilic and hydrogen bonding interactions between this class of inhibitors and the protein. We describe the correlation of the structure-activity relationships and crystallog. structures of these inhibitors with p38. In addition, we incorporated another binding pharmacophore that forms a hydrogen bond at the ATP binding site. This modification affords significant improvements in binding, cellular, and in vivo potencies resulting in the selection of Compound 45 (BIRB 796) as a clin. candidate for the treatment of inflammatory diseases.

RX(7) OF 99



REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 24 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 135:211001 CASREACT

TITLE: A new and efficient approach to the synthesis of 6-amidino-2-oxopurines

AUTHOR(S): Booth, Brian L.; Cabral, Isabel M.; Dias, Alice M.; Freitas, A. Paula; Matos Beja, Ana M.; Proenca, M. Fernanda; Silva, Manuela Ramos

CORPORATE SOURCE: Department of Chemistry, UMIST, Manchester, M60 1QD, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions 1 (2001), (10), 1241-1251

CODEN: JCSPCE; ISSN: 1472-7781

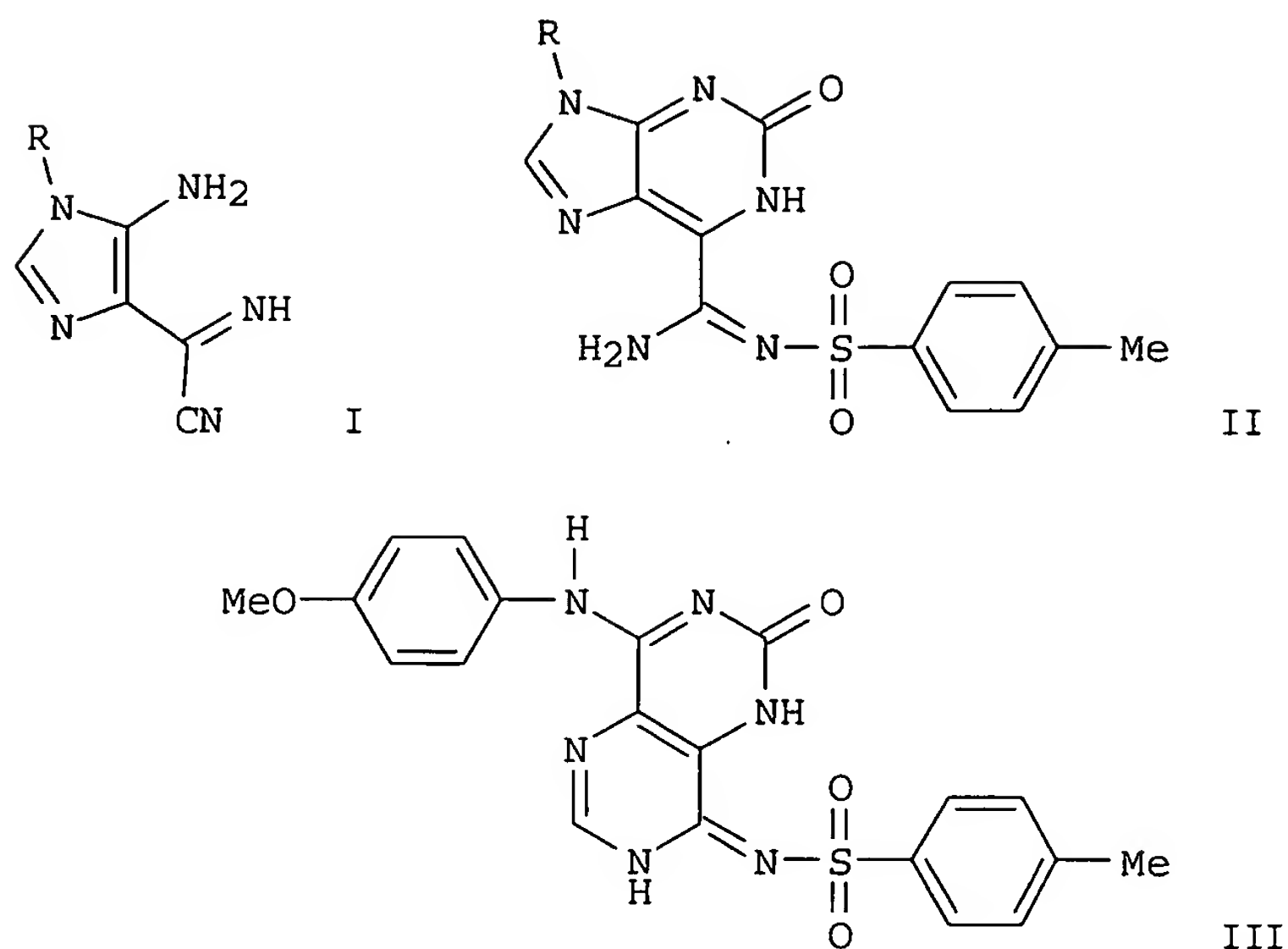
PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



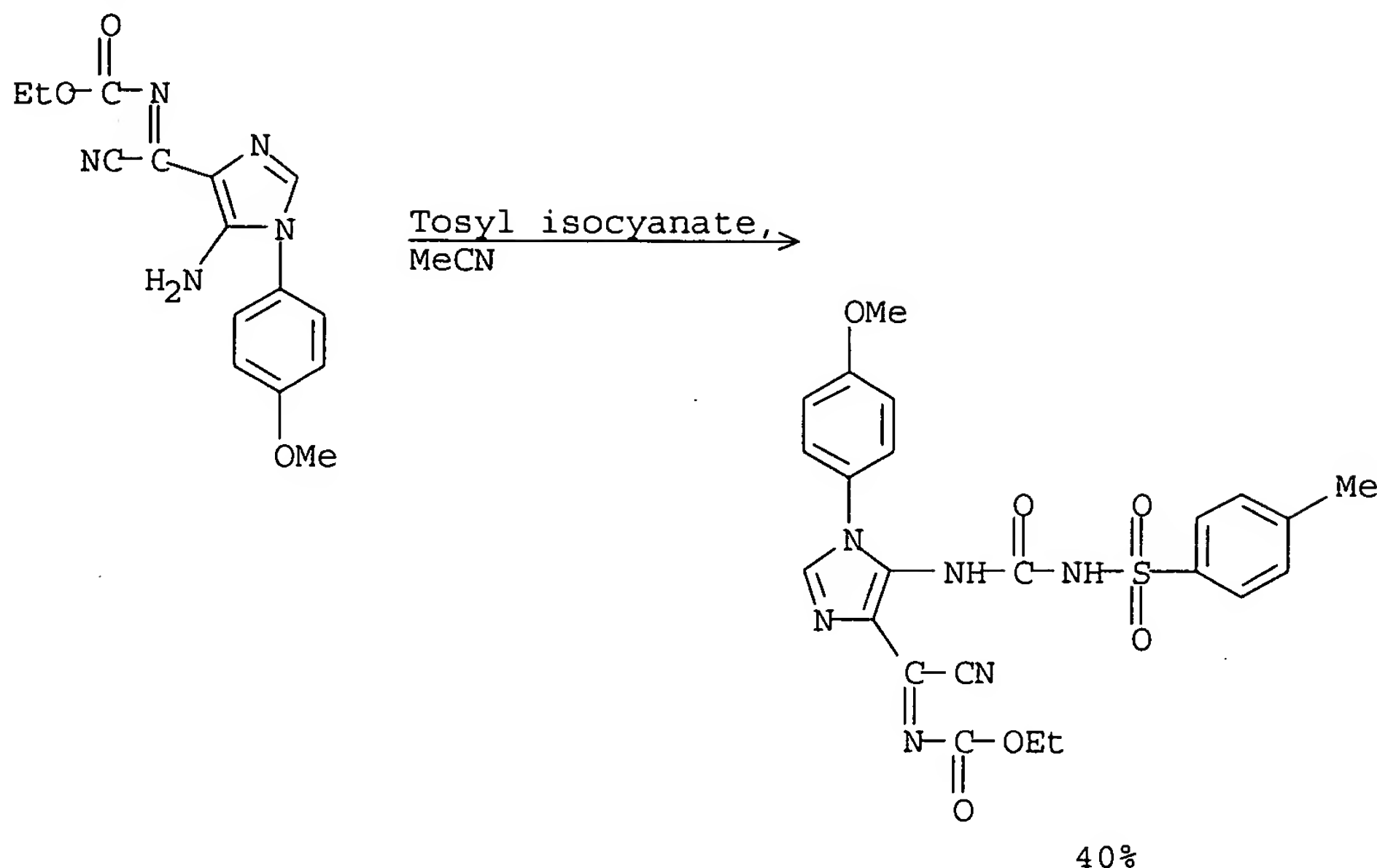


AB The reaction of 5-amino-4-cyanoformimidoylimidazoles I ( $R = \text{HOCH}_2\text{CH}_2$ , 4-MeOC<sub>6</sub>H<sub>4</sub>) with tosyl isocyanate proved to be a mild and efficient method for the synthesis of the corresponding 6-amidino-2-oxopurines II. These compds., which were isolated in almost quant. yield, rearrange in the presence of acetic acid-DMF to give a pyrimido[5,4-d]pyrimidin-2-one, e.g. III. The structure of compound III was confirmed by X-ray crystallog. The pathway for both reactions is discussed. Studies on the reactivity of tosyl isocyanate with imidazoles derived from I by selective acylation of the amino or imino nitrogen atoms, enabled clarification of the mechanism for purine formation.



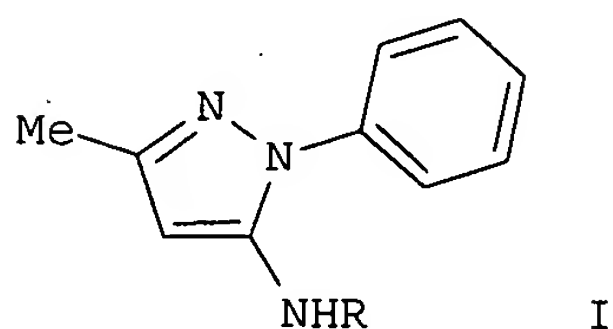
10/074,895

RX(21) OF 41



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

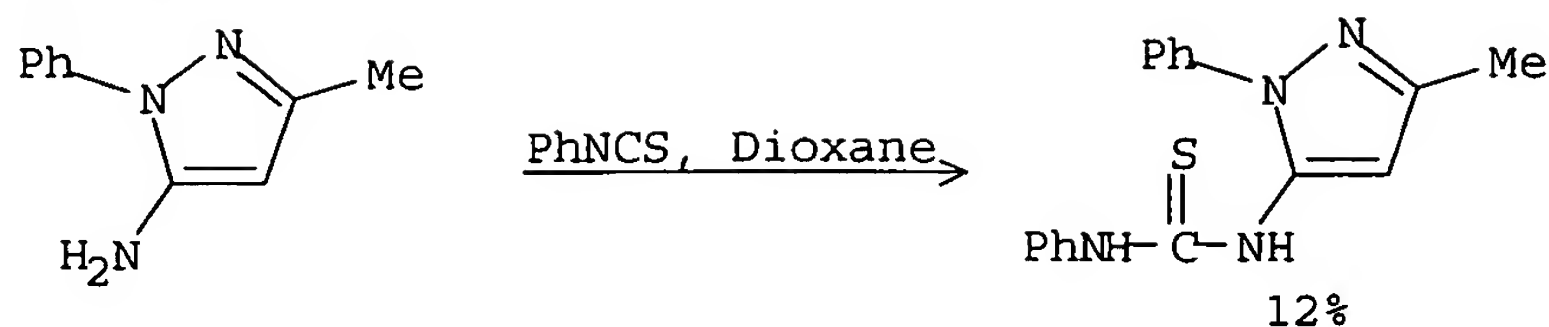
L3 ANSWER 8 OF 24 CASREACT COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 134:340456 CASREACT  
TITLE: Synthesis of N-acyl derivatives of  
1-phenyl-3-methyl-5-aminopyrazole  
AUTHOR(S): Nam, N. L.; Grandberg, I. I.; Sorokin, V. I.  
CORPORATE SOURCE: Kafedra Org. Khim., Mosk. S-Kh. Akad. im. K. A.  
Timiryazeva, Moscow, Russia  
SOURCE: Izvestiya Timiryazevskoi Sel'skokhozyaistvennoi  
Akademii (2000), (1), 172-176  
CODEN: ITSAA7; ISSN: 0021-342X  
PUBLISHER: Izdatel'stvo MSKhA  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian  
GI



AB Aminopyrazole I (R = H), prepared from  $\text{PhNHNH}_2 \cdot \text{HCl}$  and  $\text{MeC:NHCH}_2\text{CN}$ , was N-acylated to give pyrazoles I (R = MeCO, PhCO, 4-ClC<sub>6</sub>H<sub>4</sub>CO, 4-BrC<sub>6</sub>H<sub>4</sub>CO, 4-MeC<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>, PhNHCO, PhNHCS) in 47-78% yields.

10/074,895

RX(5) OF 15



L3 ANSWER 9 OF 24 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 134:237742 CASREACT

TITLE: Synthesis of sugar-modified derivatives of the unusual nucleoside oxanosine and its carbocyclic analogs as potential inhibitors of HIV

AUTHOR(S): Saito, Yoshio; Nakamura, Mariko; Ohno, Tsuneya; Chaicharoenpong, Chanya; Ichikawa, Eiko; Yamamura, Shosuke; Kato, Kuniki; Umezawa, Kazuo

CORPORATE SOURCE: Departments of Applied Chemistry and Chemistry, Keio University, Kohoku-ku, Yokohama, 223-0061, Japan

SOURCE: Journal of the Chemical Society, Perkin Transactions 1 (2001), (3), 298-304

CODEN: JCSPCE; ISSN: 1472-7781

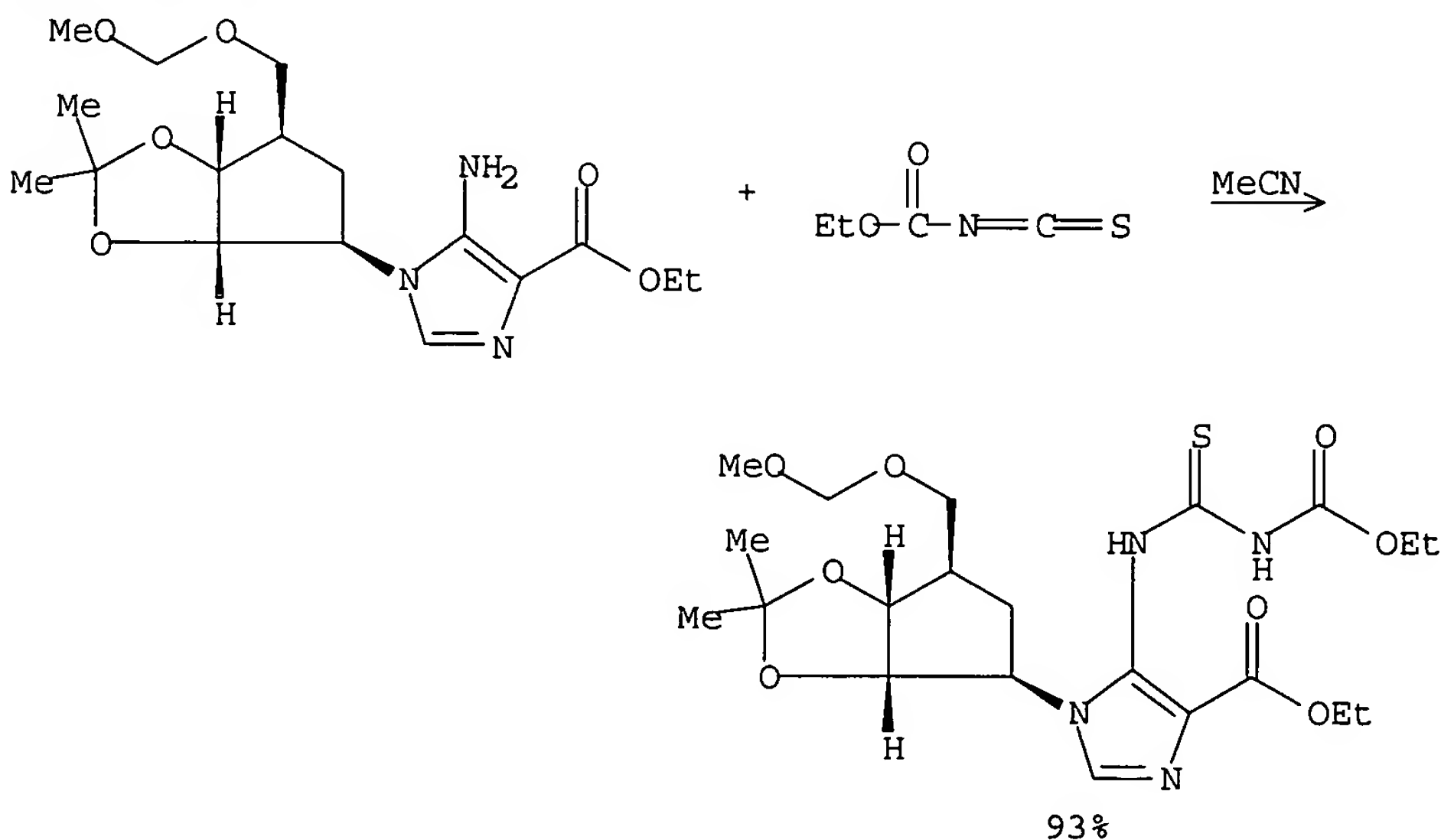
PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of sugar-modified derivs. of oxanosine and its carbocyclic analogs were synthesized from natural oxanosine and (-)-2-azabicyclo[2.2.1]hept-5-en-3-one, resp. Among nucleosides tested for anti-HIV activities in vitro, oxanosine, its 5'-monophosphate, and 2'-deoxyoxanosine reduced the number of HIV particles in CEM cells to almost the same level as ddI.

RX(9) OF 52



NOTE: stereoselective

REFERENCE COUNT:

15

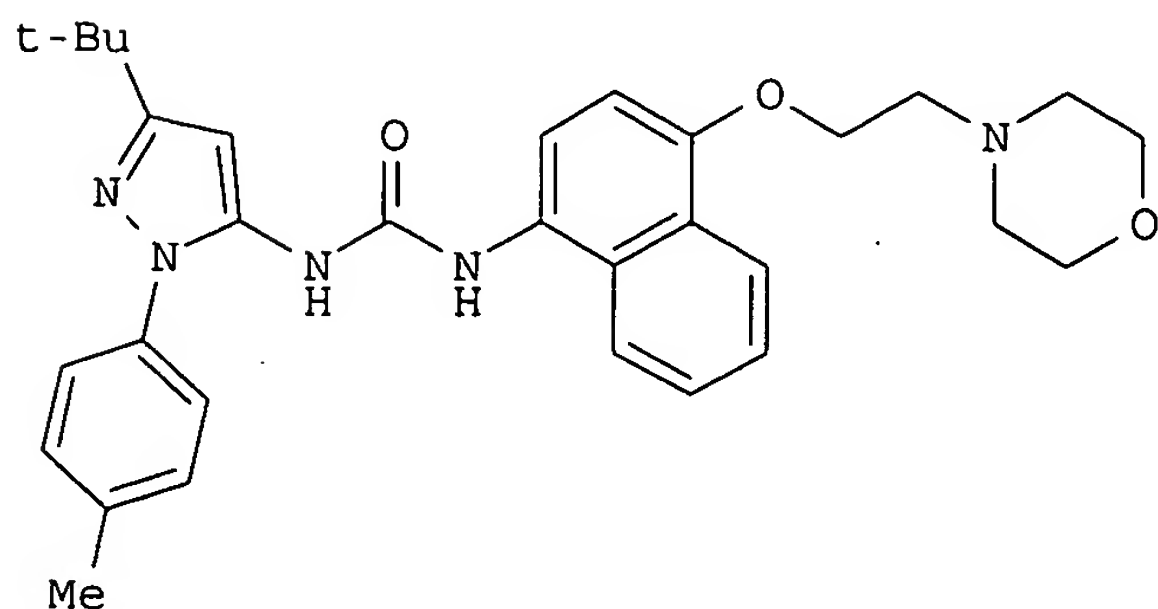
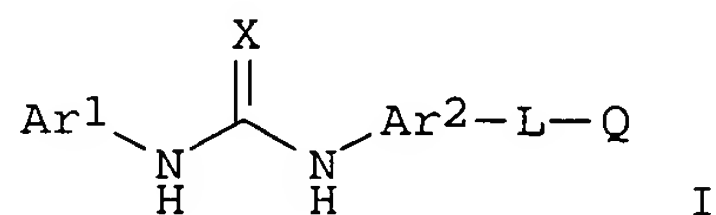
THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/074,895

L3 ANSWER 10 OF 24 CASREACT COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 134:86264 CASREACT  
TITLE: Novel process for synthesis of heteroaryl-substituted ureas  
INVENTOR(S): Zhang, Lin-Hua; Zhu, Lei  
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA  
SOURCE: PCT Int. Appl., 37 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001004115	A2	20010118	WO 2000-US17655	20000627
WO 2001004115	A3	20010927		
W: CA, JP, MX				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2374737	AA	20010118	CA 2000-2374737	20000627
EP 1200411	A2	20020502	EP 2000-941745	20000627
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
JP 2003504366	T2	20030204	JP 2001-509725	20000627
US 6583282	B1	20030624	US 2000-611109	20000706
US 2003109703	A1	20030612	US 2002-300448	20021120
US 6753426	B2	20040622		
US 2003166930	A1	20030904	US 2003-361719	20030210
US 6774233	B2	20040810		
US 2003166931	A1	20030904	US 2003-361731	20030210
US 6835832	B2	20041228		
US 2003181718	A1	20030925	US 2003-361440	20030210
PRIORITY APPLN. INFO.:				
			US 1999-143094P	19990709
			WO 2000-US17655	20000627
			US 2000-611109	20000706

OTHER SOURCE(S): MARPAT 134:86264  
GI



10/074,895

AB The title compds. [I; Ar1 = (un)substituted Ph, pyridinyl, pyrazolyl, etc.; Ar2 = (un)substituted Ph, naphthyl, quinolinyl, etc.; L = alkylene wherein one or more methylene groups are optionally replaced by O, N, or S, and substituted with 0-2 oxo groups and one or more alkyl, or L = cycloalkyl or cycloalkenyl optionally substituted with 1-2 oxo, 1-3 alkyl, alkoxy, alkylamino, etc., Q = (un)substituted Ph, naphthyl, pyridinyl, etc.; X = O, S], useful in pharmaceutic compns. for treating diseases or pathol. conditions involving inflammation such as chronic inflammatory diseases (no data), were prepared E.g., a multi-step synthesis of the urea II was given.

RX(7) OF 9 - REACTION DIAGRAM NOT AVAILABLE

L3 ANSWER 11 OF 24 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 120:324107 CASREACT

TITLE: A novel synthesis of oxanosine and 1-thiaguanosine

AUTHOR(S): Luk, Kin Chun; Moore, Douglas W.; Keith, Dennis D.

CORPORATE SOURCE: Roche Res. Cent., Hoffmann-La Roche Inc., Nutley, NJ, 07110, USA

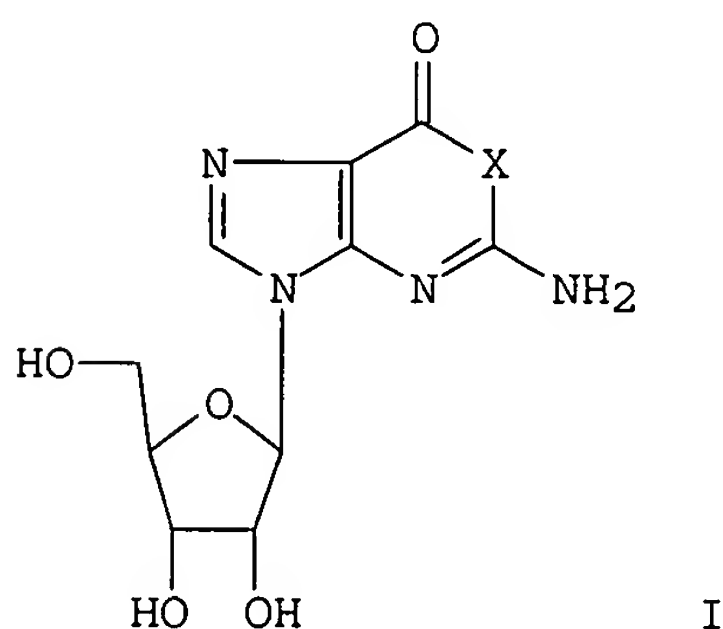
SOURCE: Tetrahedron Letters (1994), 35(7), 1007-10

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

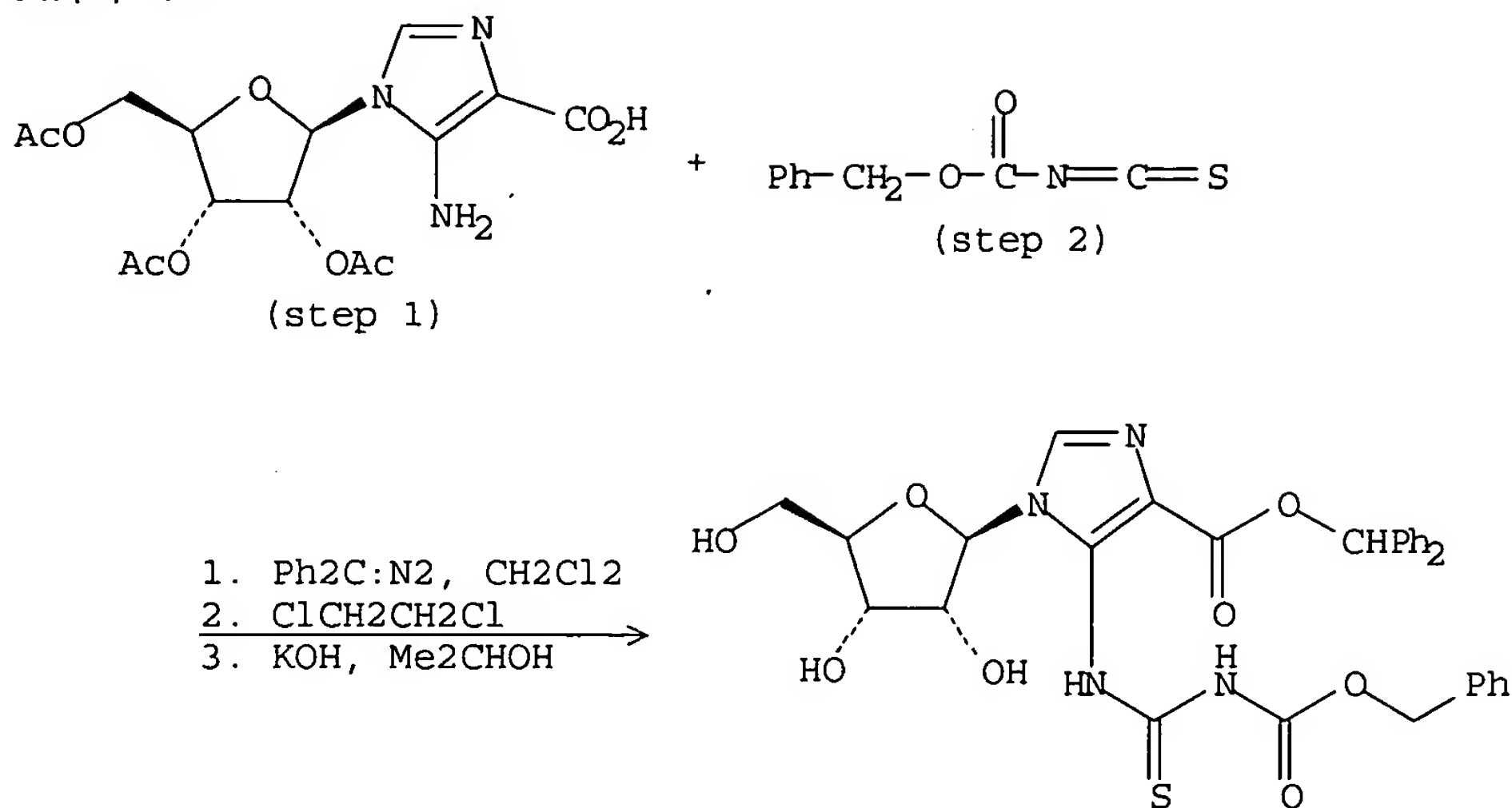
LANGUAGE: English

GI

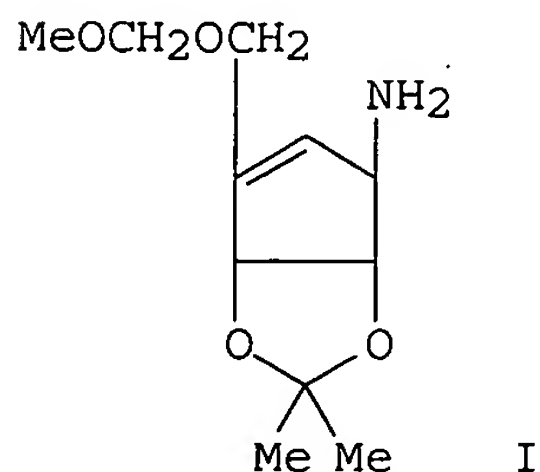


AB A novel total synthesis of oxanosine I (X = O) has been developed. The key heterocycle forming reaction of this synthesis is the carbodiimide mediated dehydration and cyclization of an urea-acid derived from AICA-riboside. The same procedure was also applied to the synthesis of 1-thiaguanosine I (X = S). Antimicrobial activity of I against E. coli 257 was completely reversed by guanosine (no data).

RX(2) OF 6



L3 ANSWER 12 OF 24 CASREACT COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 109:38166 CASREACT  
 TITLE: Enantioselective synthesis of new analogs of neplanocin A and their biological activity  
 AUTHOR(S): Arita, Masafumi; Okumoto, Takeki; Saito, Tadamasa; Hoshino, Yukio; Fukukawa, Kiyofumi; Shuto, Satoshi; Tsujino, Masatoshi; Sakakibara, Hideo; Ohno, Masaji  
 CORPORATE SOURCE: Res. Lab., Yoshitomi Pharm. Ind., Ltd., Iruma, 358, Japan  
 SOURCE: Carbohydrate Research (1987), 171, 233-58  
 CODEN: CRBRAT; ISSN: 0008-6215  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Various carbocyclic nucleosides analogs of neplanocin A; such as 5-aminoimidazole-4-carboxamide, riboside, uridine, 5-iodouridine, 4-thiouridine, cytidine, thymidine, 2'-deoxyguanosine, ribofuranosylthymine, a 2,2'-anhydroderivative, 2'-deoxycytidine, 2'-deoxythiouridine, and D-arabinofuranosylcytosine analogs were prepared from (1R,2S,3R)-2,3-isopropylidenedioxy-4-methoxymethoxymethyl-4-cyclopenten-1-ylamine (I). The cytidine analog was found the most active in inhibiting mouse lymphoma L5178Y cells in vitro at a concentration as low as 0.8  $\mu\text{g/mL}$ .

10/074,895

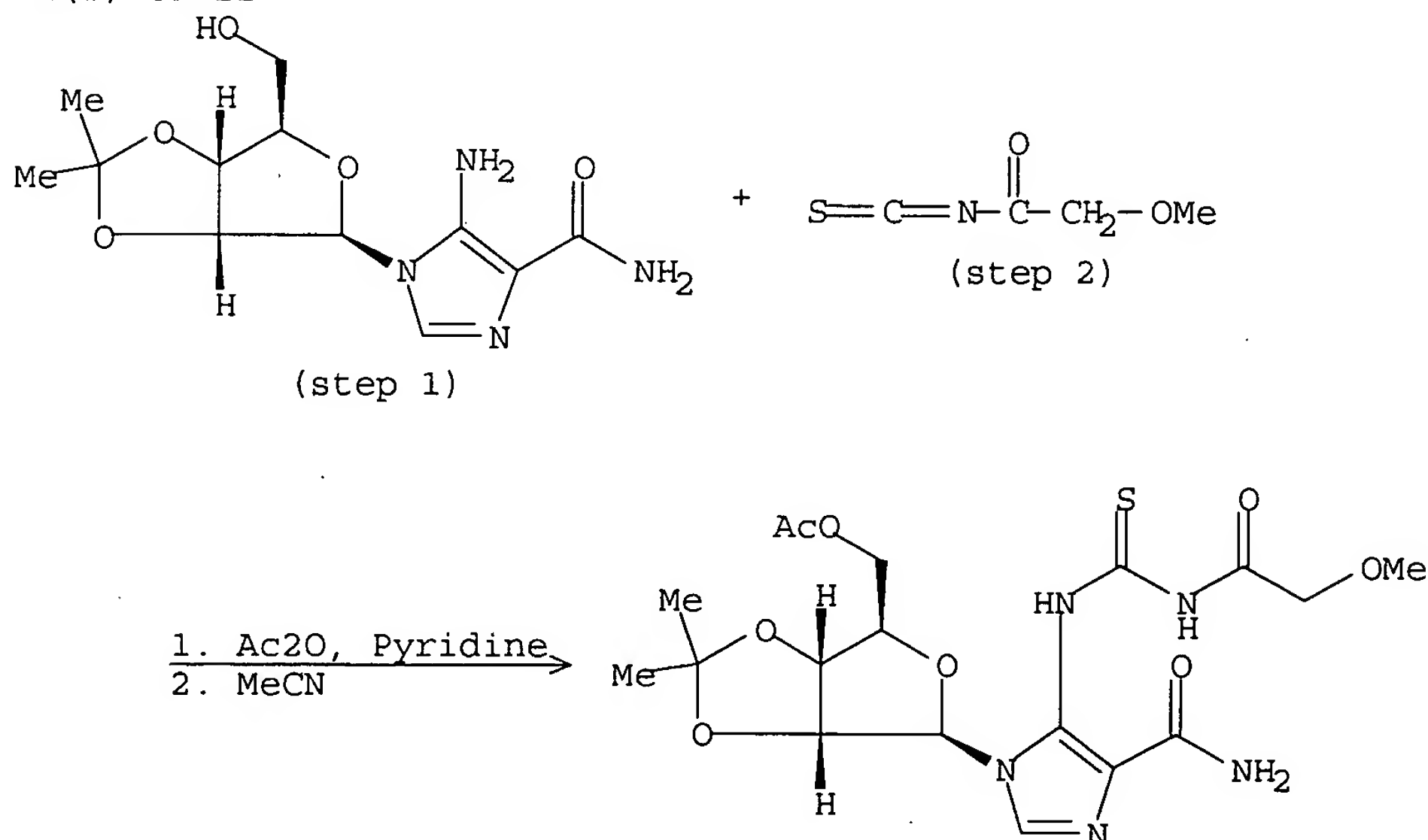
RX(3) OF 378 - REACTION DIAGRAM NOT AVAILABLE

L3 ANSWER 13 OF 24 CASREACT COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 108:150875 CASREACT  
TITLE: Conversion of the 2',3'-O-isopropylidene derivative of  
5-amino-1-β-D-ribofuranosylimidazole-4-  
carboxamide (AICA riboside) into 2',3'-O-  
isopropylideneisoguanosine  
AUTHOR(S): Reese, Colin B.; Sanghvi, Yogesh S.; Kuroda, Reiko  
CORPORATE SOURCE: Dep. Chem., King's Coll., London, WC2R 2LS, UK  
SOURCE: Journal of the Chemical Society, Perkin Transactions  
1: Organic and Bio-Organic Chemistry (1972-1999)  
(1987), (7), 1527-31  
CODEN: JCPRB4; ISSN: 0300-922X  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

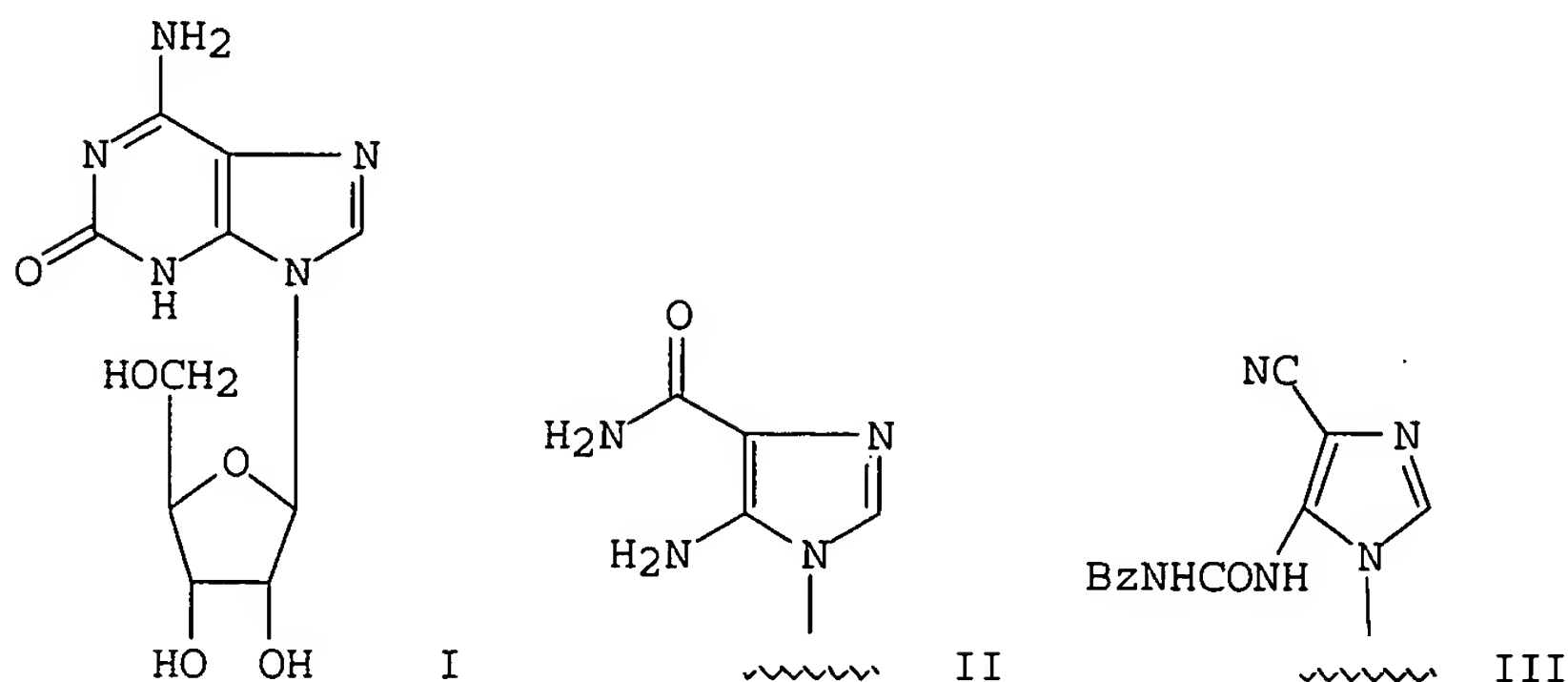
AB Treatment of the putative methoxyacetylthioureido derivative I (R = COCH<sub>2</sub>OMe), which was prepared in 2 steps from 5-amino-1-(2',3'-O-isopropylidene-β-D-ribofuranosyl)imidazole-4-carboxamide, with Hg(ClO<sub>4</sub>)<sub>2</sub> in the presence of pyridine in THF at room temperature and then with NH<sub>3</sub>-MeOH gives the ureido nitrile II (R = H) (III); treatment of I (R = H) with Hg<sup>2+</sup> under the same conditions gives II (R = Ac). When III is allowed to react with (Me<sub>2</sub>N)2C:NH and H<sub>2</sub>O in THF at room temperature, 2',3'-O-isopropylideneisoguanosine (IV) is obtained in high yield; however, when III is heated, under reflux, with Et<sub>3</sub>N in dioxane-water, 5-amino-1-(2',3'-O-isopropylidene-β-D-ribofuranosyl)imidazole-4-carbonitrile is obtained in good yield.

RX(2) OF 22



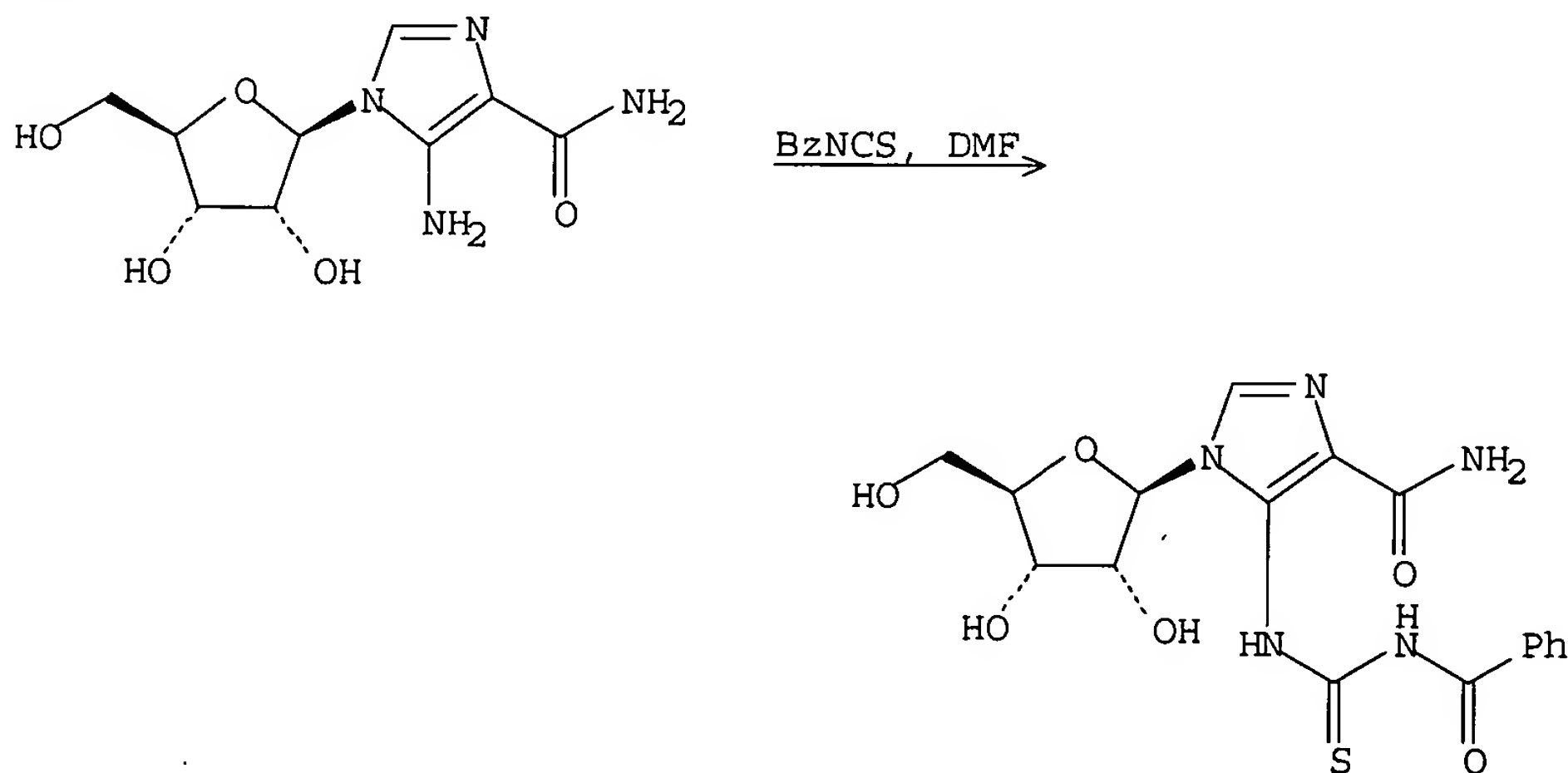
10/074,895

L3 ANSWER 14 OF 24 CASREACT COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 108:38286 CASREACT  
TITLE: Novel and efficient synthesis of isoguanosine  
AUTHOR(S): Chern, Ji Wang; Lee, Horng Yuh; Huang, Min; Shish, Fang Jy  
CORPORATE SOURCE: Med. Lab., Natl. Def. Med. Cent., Taipei, Taiwan  
SOURCE: Tetrahedron Letters (1987), 28(19), 2151-4  
CODEN: TELEAY; ISSN: 0040-4039  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Isoguanosine (I) was prepared by a one-pot reaction involving a condensation of 5-amino-1-(β-D-ribofuranosyl)imidazole-4-carboxamide (II) with benzoyl isothiocyanate, treatment of the resulting thiourea derivative with N,N'-dicyclohexylcarbodiimide furnished imidazolecarbonitrile III which was then annulated with ethanolic ammonia to afford I in a 68% yield from II.

RX(4) OF 9

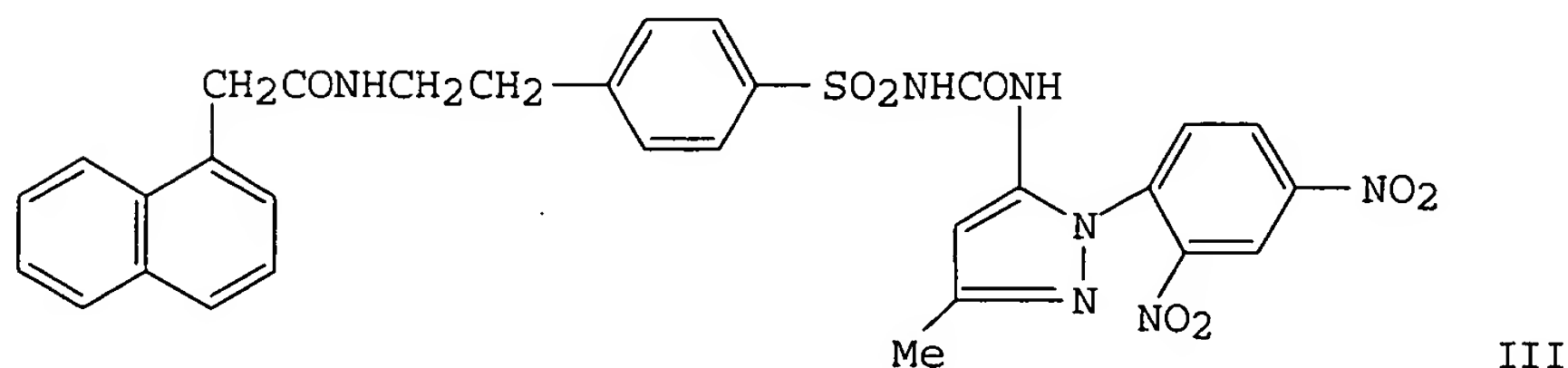
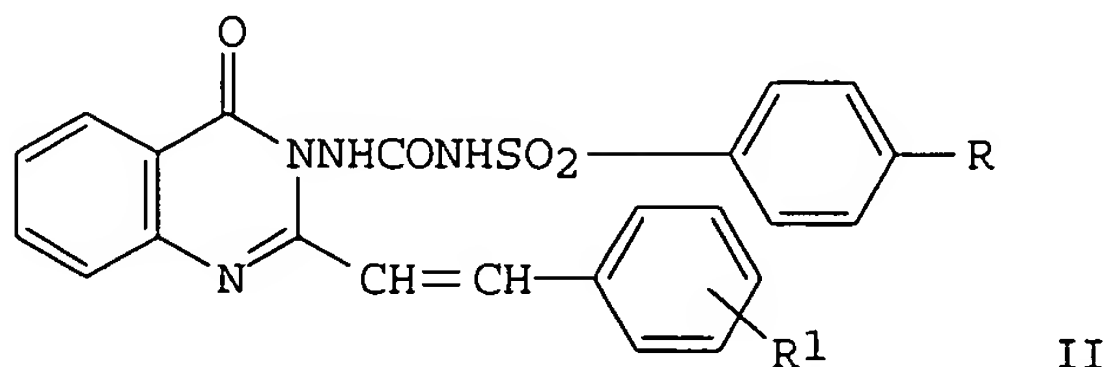
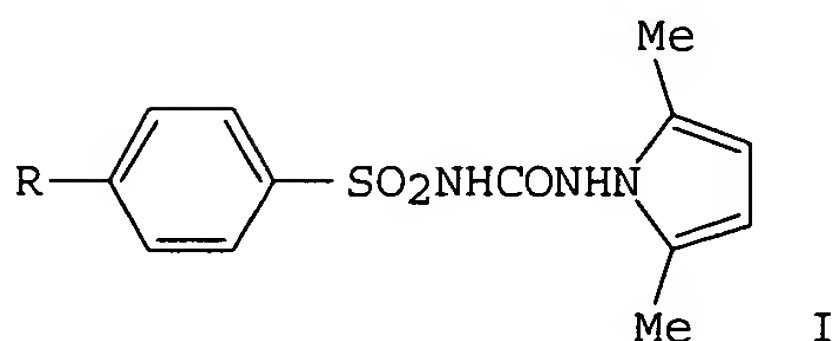


L3 ANSWER 15 OF 24 CASREACT COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 107:58968 CASREACT



10/074,895

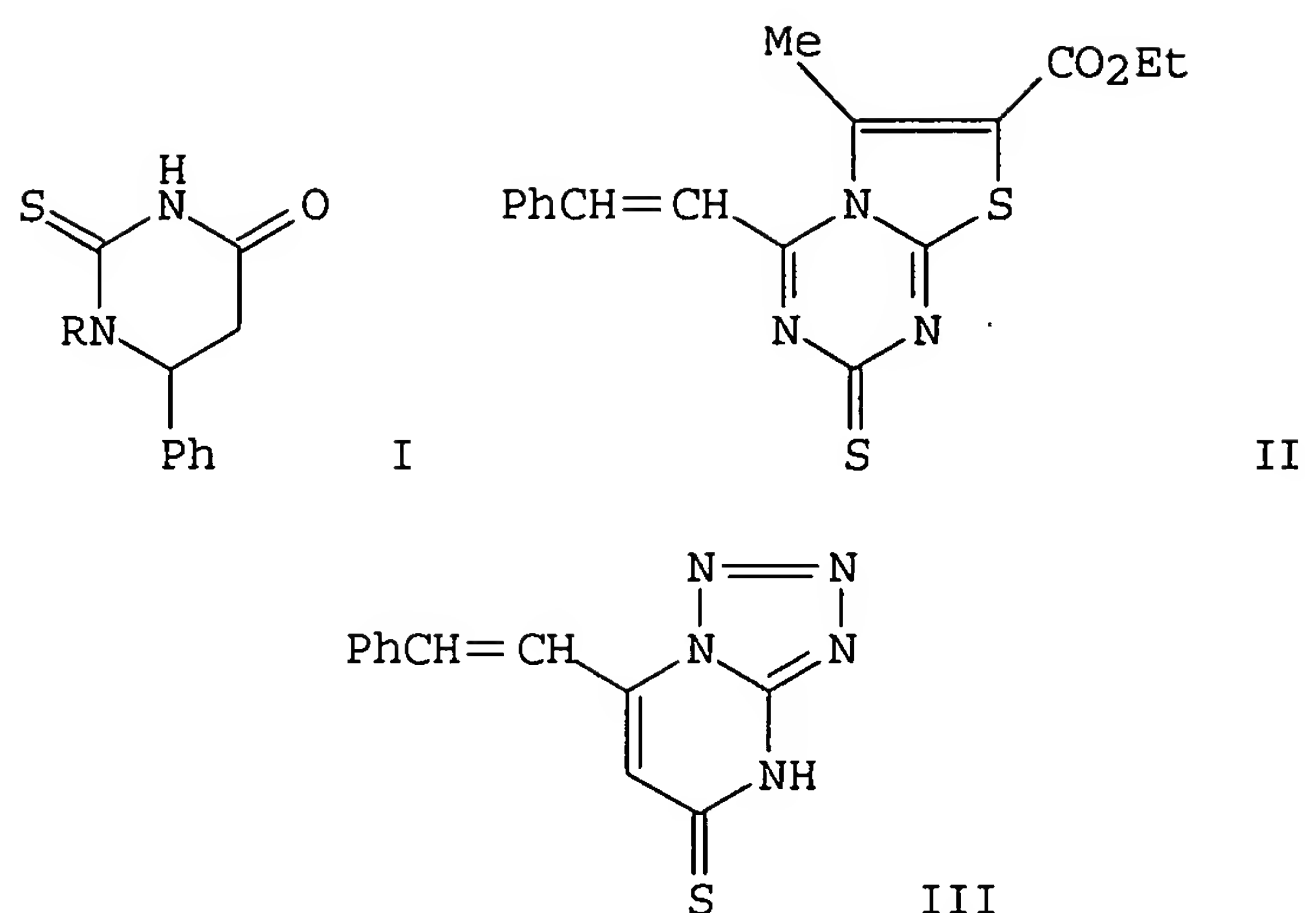
TITLE: Synthesis of some new substituted sulfonylureas as oral hypoglycemic agents  
AUTHOR(S): Husain, M. I.; Srivastava, V. P.  
CORPORATE SOURCE: Dep. Chem., Lucknow Univ., Lucknow, 226 007, India  
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1986), 25B(9), 934-8  
CODEN: IJSBDB; ISSN: 0376-4699  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB The title compds., e.g. I (R = H, Me, MeO, AcNH), II (R1 = 4-Me, 4-MeO, 4-Cl, 4-NO2) and III were prepared and their hypoglycemic activity evaluated. Some of these compds., when screened on albino rats at an oral dose of 250 mg/kg body weight, reduce the blood sugar to a significant extent.

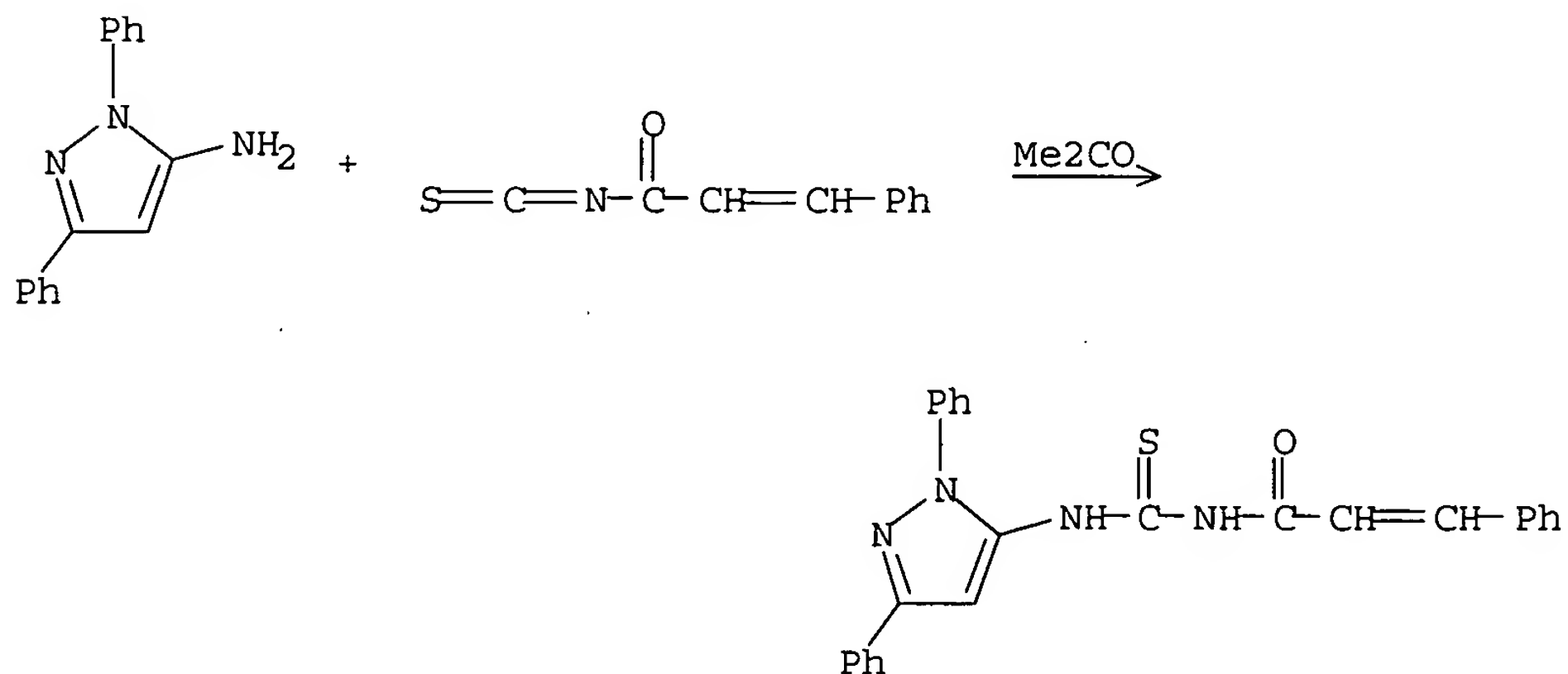
RX(36) OF 107 - REACTION DIAGRAM NOT AVAILABLE

L3 ANSWER 16 OF 24 CASREACT COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 106:119838 CASREACT  
TITLE: A new convenient synthesis of 1,6-diaryl-2-thioxoperhydro-4-pyrimidinones: reaction of 3-phenyl-2-propenoyl isothiocyanate with aromatic and heteroaromatic amines  
AUTHOR(S): Hafez, Ebtisam Abdel Aziz; Elmoghayar, Mohamed Rifaat Hamza; Ramiz, Mahmoud Mohamed Mahfouz  
CORPORATE SOURCE: Fac. Sci., Cairo Univ., Giza, Egypt  
SOURCE: Liebigs Annalen der Chemie (1987), (1), 65-7  
CODEN: LACHDL; ISSN: 0170-2041  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB PhCH:CHCON:C:S was treated with RNH<sub>2</sub> (R = Ph, p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, p-MeOC<sub>6</sub>H<sub>4</sub>, Bu, PhCH<sub>2</sub>, 1,3-diphenyl-1H-pyrazol-5-yl, 3-phenyl-1H-pyrazol-5-yl, 5-ethoxycarbonyl-4-methyl-2-thiazolyl) to give PhCH:CHCONHCSNHR; which were cyclized by treatment with EtONa to give pyrimidinones I (R = Ph, p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>, 1,3-diphenyl-1H-pyrazol-5-yl) or thiazolotriazine II. PhCH:CHCON:C:S underwent cyclization with 1H-tetrazol-5-amine to give the tetrazolotriazine III.

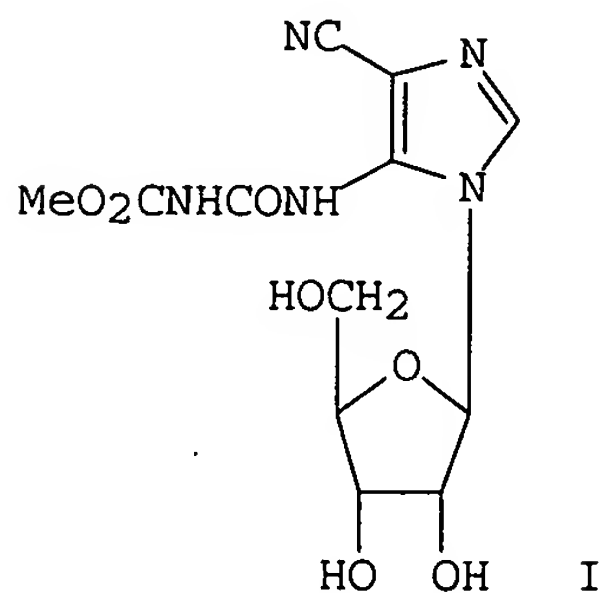
RX (6) OF 21



L3 ANSWER 17 OF 24 CASREACT COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 105:60888 CASREACT  
TITLE: An unexpected product from the cyclodesulfurization of  
5-[1-(3-methoxycarbonyl)thioureido]-1-( $\beta$ -D-  
ribofuranosyl)imidazole-4-carboxamide with  
dicyclohexylcarbodiimide  
AUTHOR(S): Chern, Ji Wang; Groziak, Michael P.; Townsend, Leroy

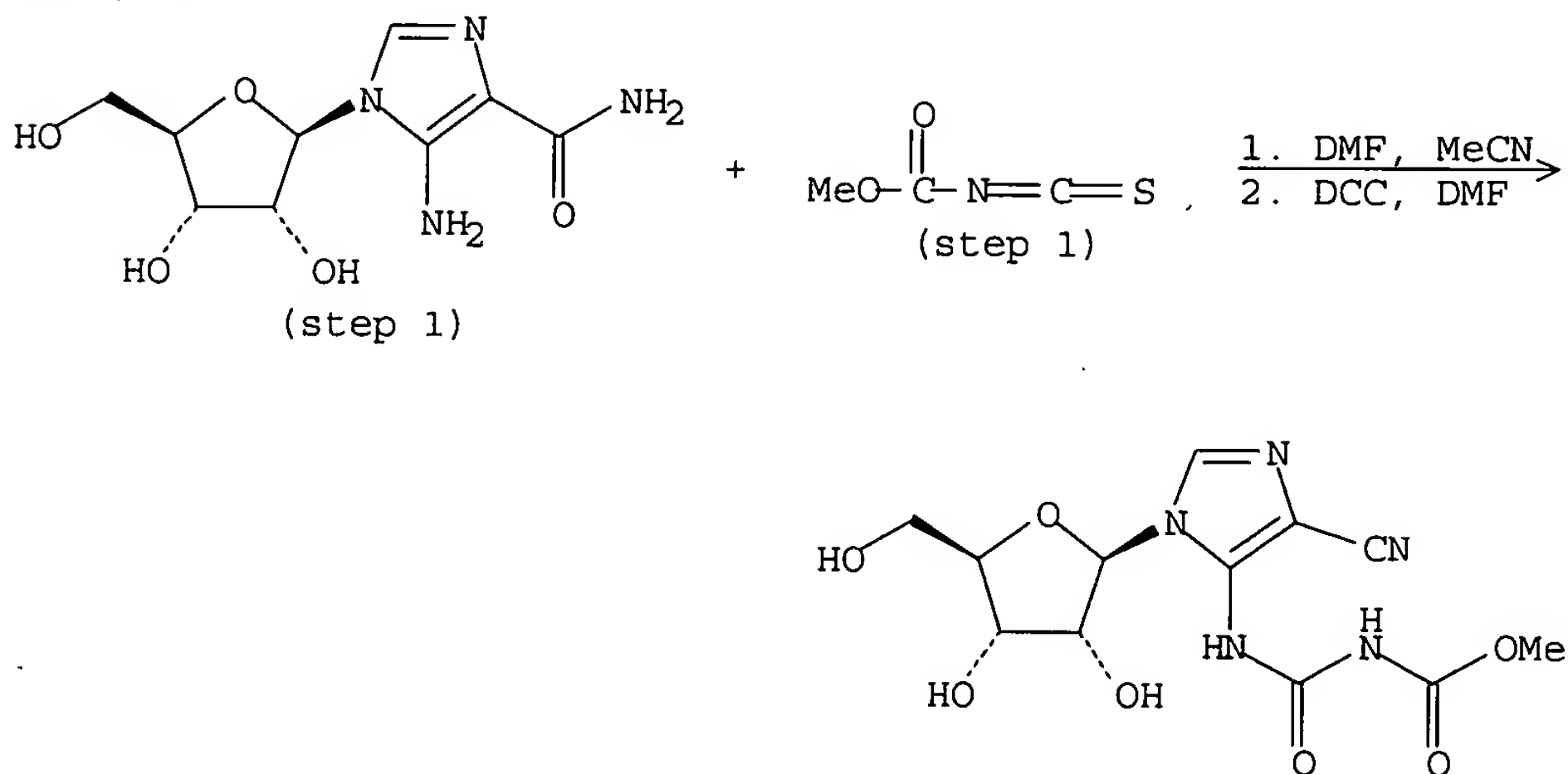
10/074,895

CORPORATE SOURCE: B.  
Coll. Pharm., Univ. Michigan, Ann Arbor, MI,  
48109-1065, USA  
SOURCE: Journal of Heterocyclic Chemistry (1986), 23(1), 153-4  
CODEN: JHTCAD; ISSN: 0022-152X  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB The treatment of 5-[1-(3-methoxycarbonyl)thioureido]-1-(β-D-ribofuranosyl)imidazole-4-carboxamide with N,N'-dicyclohexylcarbodiimide in DMF gave 4-cyano-5-[1-(3-methoxycarbonyl)-ureido]-1-(β-D-ribofuranosyl)imidazole (I).

RX(1) OF 1



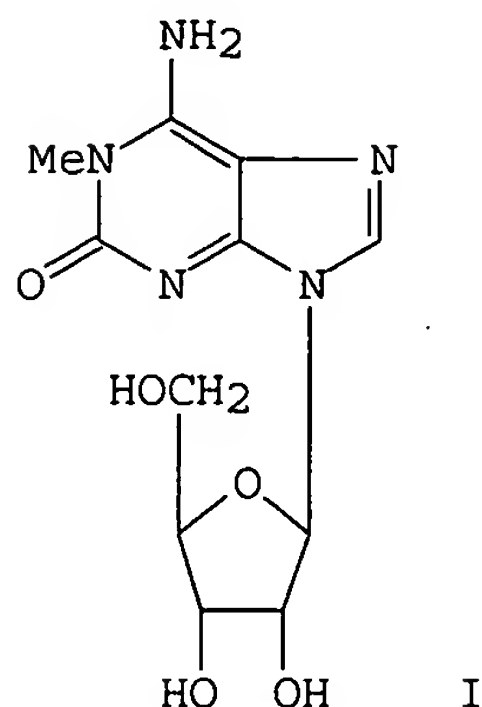
L3 ANSWER 18 OF 24 CASREACT COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 105:60880 CASREACT  
TITLE: A novel and efficient synthesis of the naturally occurring nucleoside doridosine  
AUTHOR(S): Chern, Jiwang; Townsend, Leroy B.  
CORPORATE SOURCE: Coll. Pharm., Univ. Michigan, Ann Arbor, MI,  
48109-1065, USA  
SOURCE: Tetrahedron Letters (1985), 26(52), 6419-22

10/074,895

CODEN: TELEAY; ISSN: 0040-4039

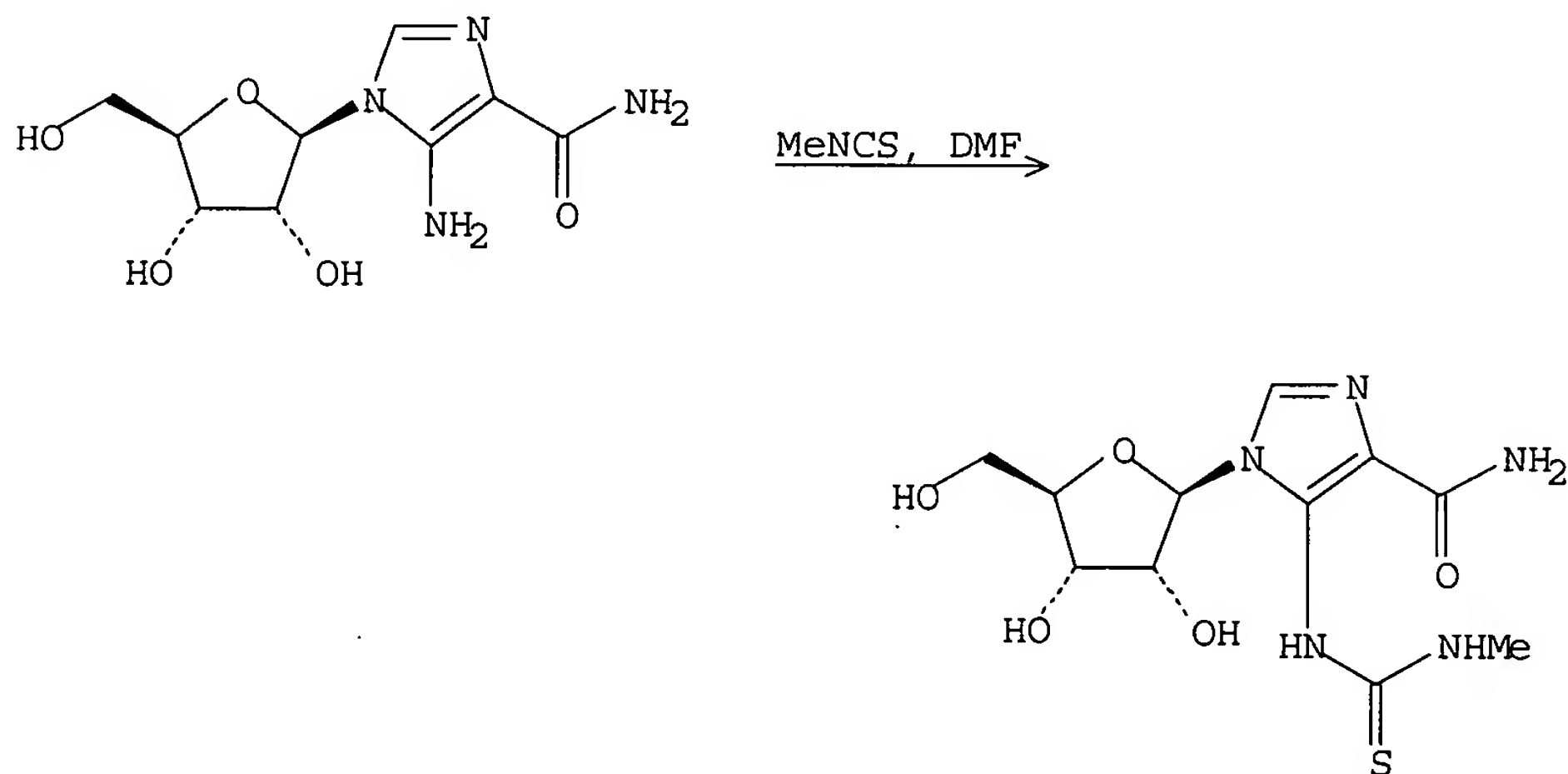
DOCUMENT TYPE:  
LANGUAGE:  
GI

Journal  
English



AB 1-Methylisoguanosine (doridosine, I) was prepared by a one-pot reaction involving a condensation of 5-amino-1-( $\beta$ -D-ribofuranosyl)imidazole-4-carboxamide (II) with Me isothiocyanate, treatment of the resulting thiourea derivative with DCC furnished 5-(3-methyl-1-ureido)-1-( $\beta$ -D-ribofuranosyl)imidazole-4-carbonitrile which was then annulated with ethanolic ammonia to furnish doridosine in a 68% yield from II.

RX(1) OF 3

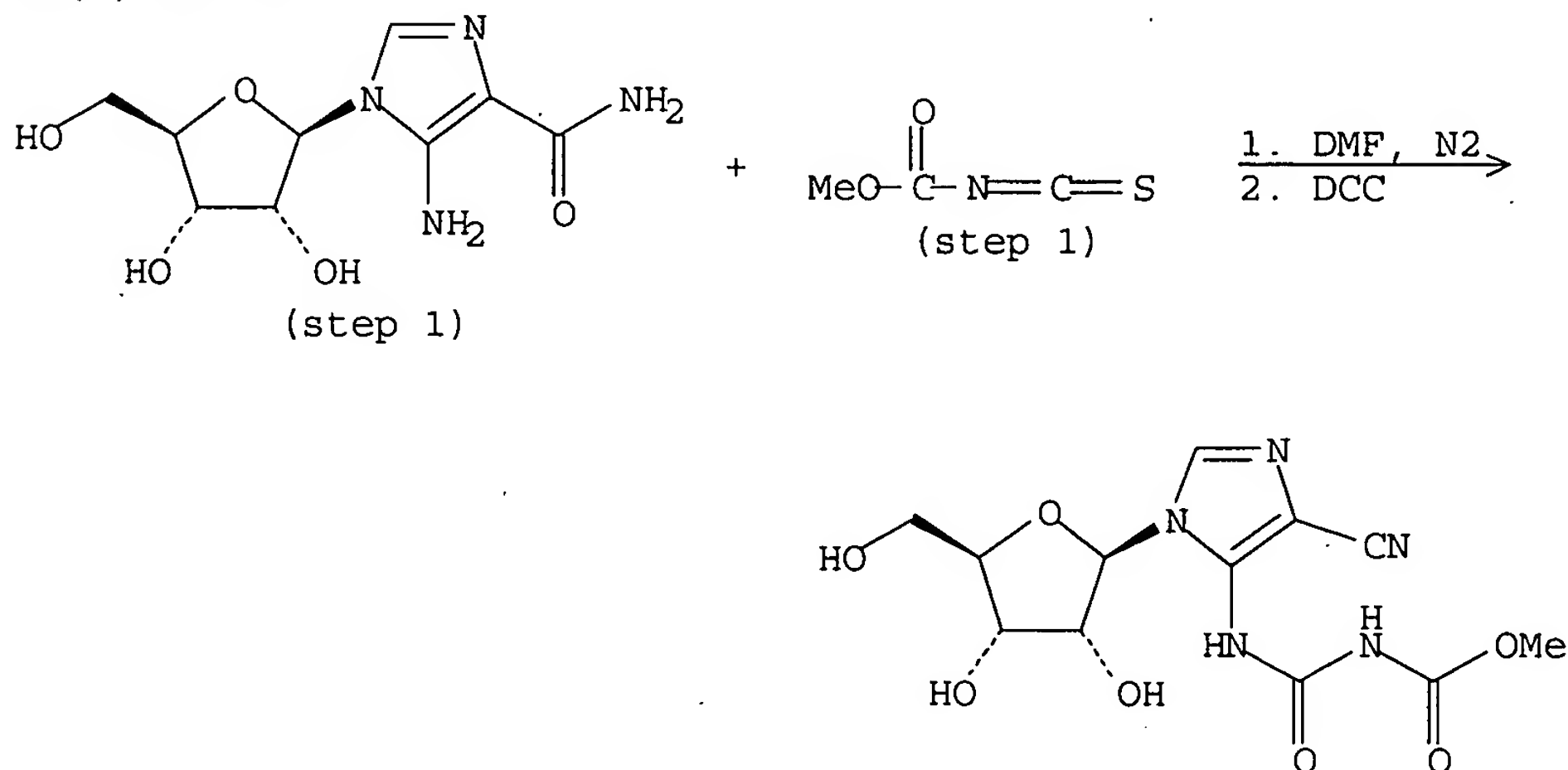


L3 ANSWER 19 OF 24 CASREACT COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 104:149337 CASREACT  
TITLE: Heterocyclic synthesis via a 1,3-dicyclohexylcarbodiimide-mediated cyclodesulfurative annulation reaction. New methodology for the preparation of guanosine and guanosine-type nucleoside analogs  
AUTHOR(S): Groziak, Michael P.; Chern, Ji Wang; Townsend, Leroy

10/074,895

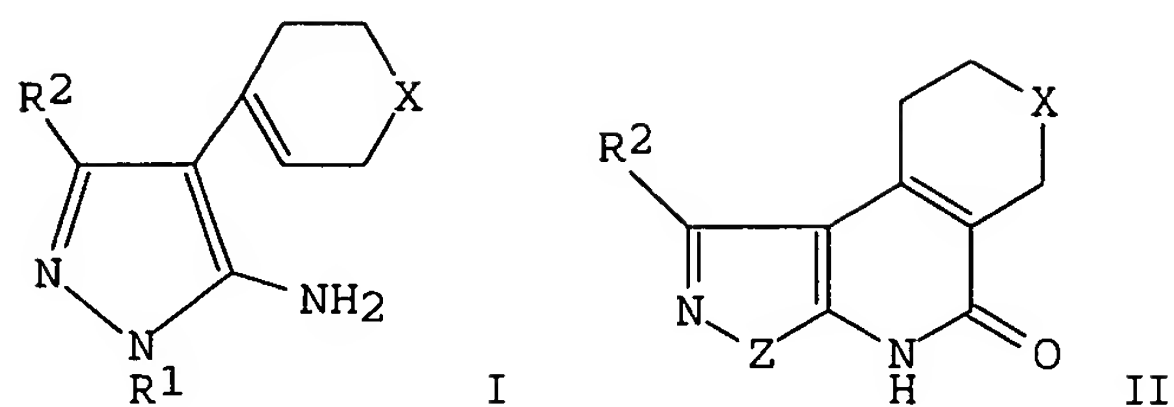
CORPORATE SOURCE: B.  
Coll. Pharm., Univ. Michigan, Ann Arbor, MI,  
48109-1065, USA  
SOURCE: Journal of Organic Chemistry (1986), 51(7), 1065-9  
CODEN: JOCEAH; ISSN: 0022-3263  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI For diagram(s), see printed CA Issue.  
AB Treatment of aminoribofuranosylimidazolecarboxamide (I, R = CONH<sub>2</sub>) with MeO<sub>2</sub>CNCS followed by cyclodesulfurization with DCC furnished [(methoxycarbonyl)ureido]ribofuranosylimidazolecarbonitrile (II, X = O). II (X = O, 180) were also produced by hydrolysis of I (R = cyano) with H<sub>2</sub>1802 and NH<sub>4</sub>OH followed by amidation and cyclodesulfurization, under similar reaction conditions. Me 5-amino-1-β-D-ribofuranosylimidazole-4-carboximide affords 6-methoxy-2-[(methoxycarbonyl)amino]-9-β-D-ribofuranosylpurine, which gives guanosine upon deprotection with Me<sub>3</sub>SiI.

RX(1) OF 15



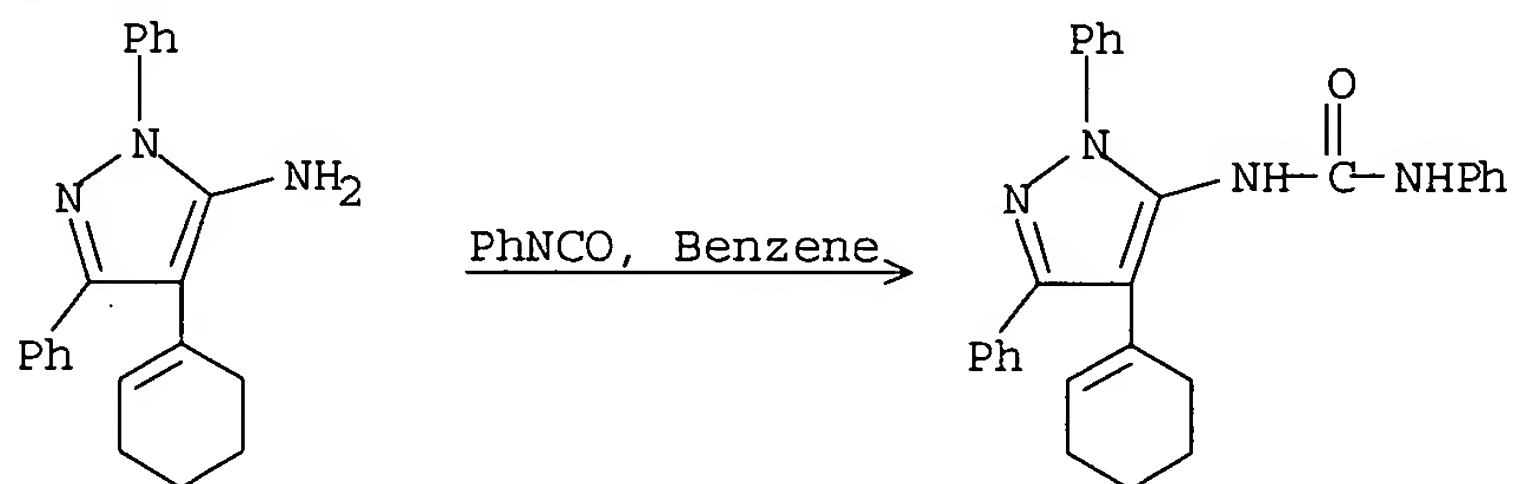
L3 ANSWER 20 OF 24 CASREACT COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 103:37407 CASREACT  
TITLE: Easy synthesis of new ring-fused pyridones from heteroaromatic β-vinylamines  
AUTHOR(S): Winters, G.; Sala, A.; De Paoli, A.; Ferri, V.  
CORPORATE SOURCE: Res. Lab., DOW-Lepetit, Milan, I-20158, Italy  
SOURCE: Synthesis (1984), (12), 1052-4  
CODEN: SYNTBF; ISSN: 0039-7881  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI

10/074,895

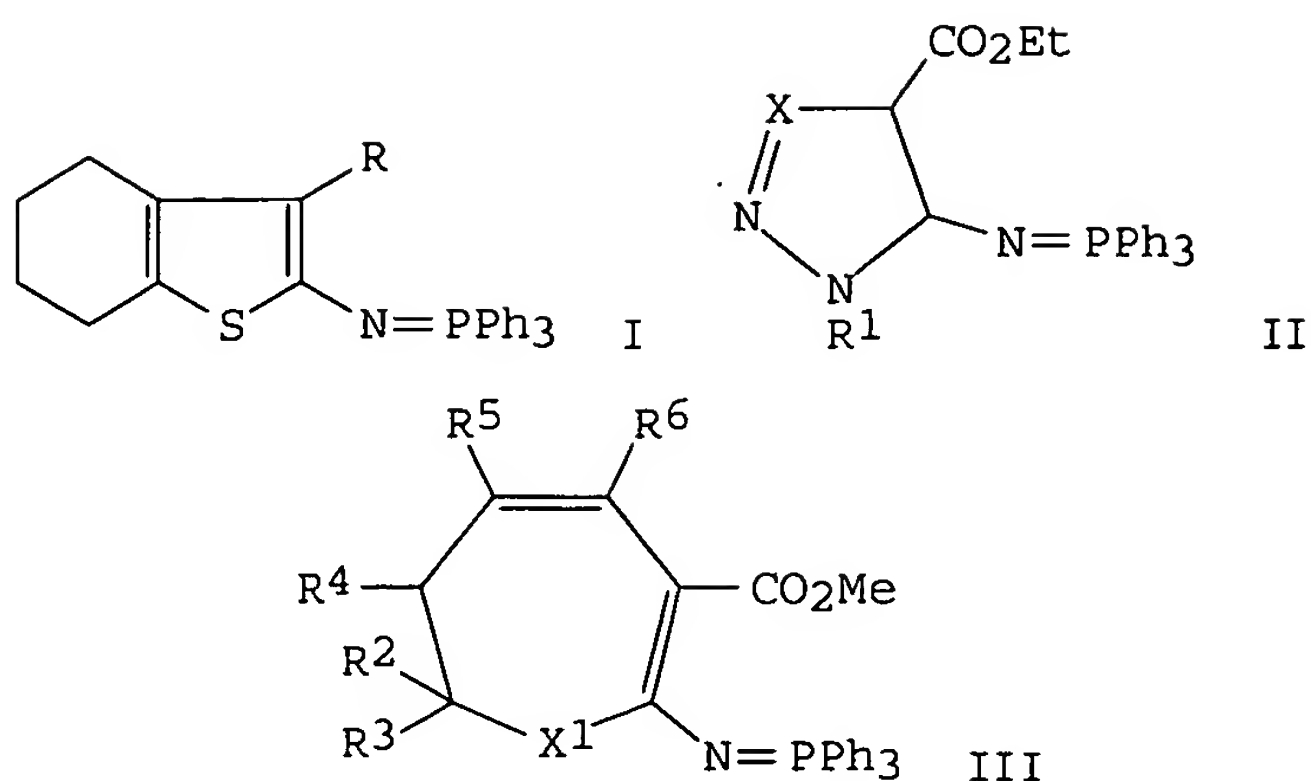


AB Cyclization of pyrazoles I ( $R_1, R_2 = \text{Me, Ph}$ ;  $X = -, \text{CH}_2, \text{CH}_2\text{CH}_2, \text{NAC, NMe}$ ) with  $\text{RNCO}$  ( $R = \text{Ph, Et}$ ) gave 75-98% cycloalkapyrazolopyridines II ( $Z = \text{NR}_1$ ). Similarly prepared were II ( $Z = \text{O}$ ).

RX(2) OF 28

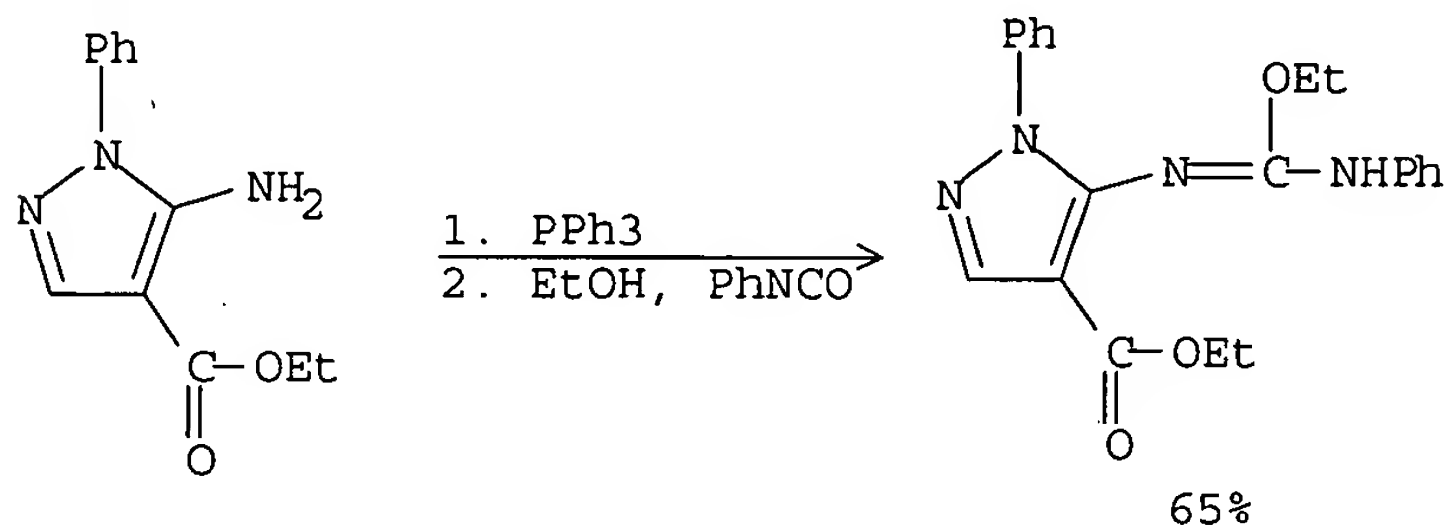


L3 ANSWER 21 OF 24 CASREACT COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 101:55022 CASREACT  
TITLE: Heterocyclic  $\beta$ -enamino esters. 31. Heterocyclic syntheses using dihalotriphenylphosphoranes. 6. New 6:7-, 6:8-, and 5:6:7-combinations of heterocondensed pyrimidines from iminophosphoranes of heterocyclic  $\beta$ -enamino esters. Stable heterocyclic ylides  
AUTHOR(S): Wamhoff, Heinrich; Haffmanns, Guenter  
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Univ. Bonn, Bonn, D-5300/1, Fed. Rep. Ger.  
SOURCE: Chemische Berichte (1984), 117(2), 585-621  
CODEN: CHBEAM; ISSN: 0009-2940  
DOCUMENT TYPE: Journal  
LANGUAGE: German  
GI



AB Tetrahydrobenzothiophenyliminophosphoranes I ( $R = \text{CO}_2\text{Et}$ , cyano), heterocyclyliminophosphoranes II ( $X = \text{CH}$ ,  $\text{N}$ ;  $R_1 = \text{H}$ ,  $\text{Ph}$ ,  $\text{Me}$ ) and oxa- or thiacycloheptadienyliminophosphoranes III ( $X_1 = \text{O}$ ,  $\text{S}$ ;  $R_2$ ,  $R_3$ ,  $R_4 = \text{H}$ ,  $\text{Me}$ ;  $R_5 = \text{CO}_2\text{Et}$ , cyano;  $R_6 = \text{CO}_2\text{Me}$ ,  $\text{H}$ ) were prepared and their addition and cyclization reactions were studied. About 50 title pyrimidines were prepared

RX(74) OF 133 - 2 STEPS



L3 ANSWER 22 OF 24 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 87:201478 CASREACT

TITLE: Synthesis and reactivity of 4,5-disubstituted 3-chloro-1,2,4-triazoles and their methylsulfonyl analogs

AUTHOR(S): Nath, T. G. Surendra; Husain, Syeda; Srinivasan, V. R.

CORPORATE SOURCE: Dep. Chem., Osmania Univ., Hyderabad, India

SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1977), 15B(4), 341-6

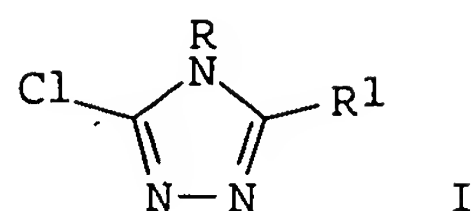
CODEN: IJSBDB; ISSN: 0376-4699

DOCUMENT TYPE: Journal

LANGUAGE: English

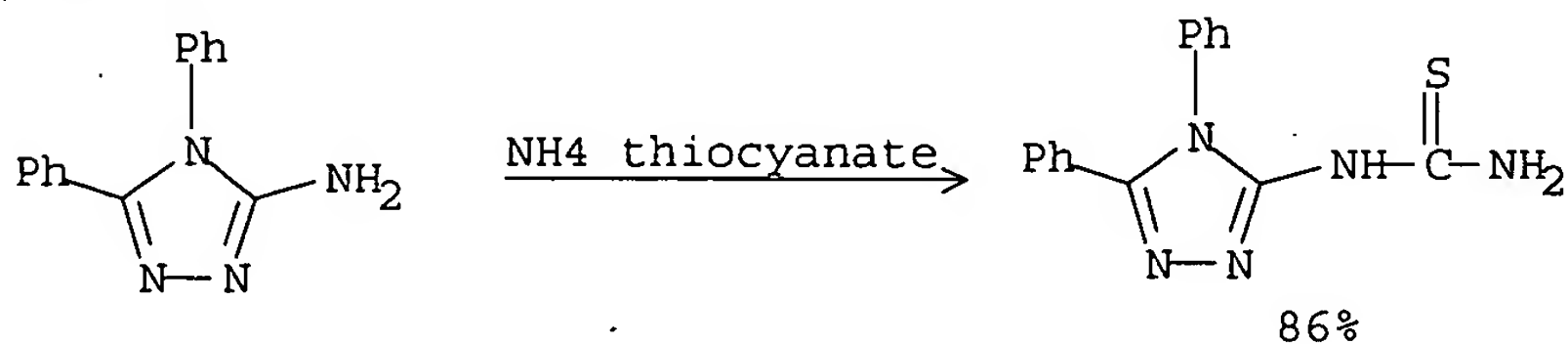
GI



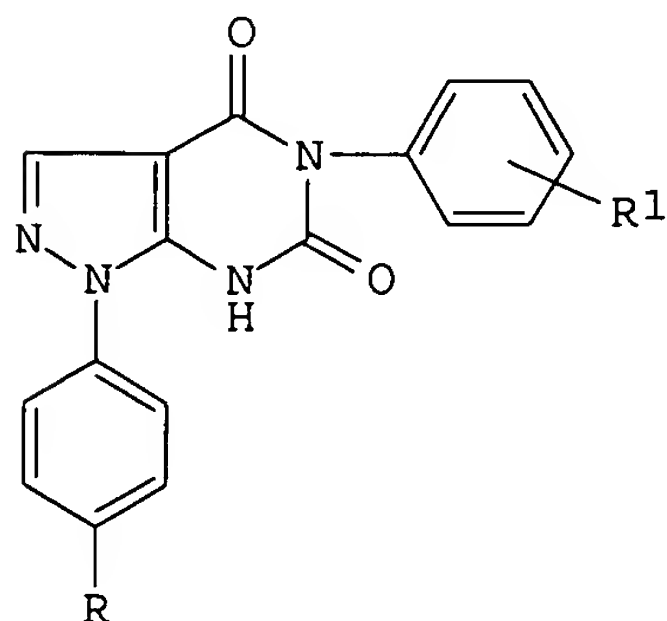


AB Several 4,5-disubstituted 3-chloro-1,2,4-triazoles I (R = Ph, 2-MeOC<sub>6</sub>H<sub>4</sub>, 2-, 3-, 4-MeC<sub>6</sub>H<sub>4</sub>; R<sub>1</sub> = Ph, 2-MeOC<sub>6</sub>H<sub>4</sub>, 5-chloro-2-thienyl, 3-pyridyl, 4-MeC<sub>6</sub>H<sub>4</sub>) were prepared either by reaction of PCl<sub>5</sub>/POCl<sub>3</sub> with the corresponding 3-hydroxytriazoles or by the oxidative chlorination of the corresponding 3-mercaptotriazoles. The Cl was replaced by H, mercapto, aryloxy, and amino groups to give variously substituted s-triazoles. The 3-methylsulfonyl analogs were prepared by the oxidation of the corresponding thioethers with KMnO<sub>4</sub> in HOAc and their reactivity studied.

RX(3) OF 21



L3 ANSWER 23 OF 24 . CASREACT COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 86:29738 CASREACT  
 TITLE: Synthesis of some derivatives of pyrazolo[3,4-d]pyrimidine-4,6-diones  
 AUTHOR(S): Sarangan, S.; Somasekhara, S.  
 CORPORATE SOURCE: Med. Chem. Div., Sarabhai Res. Cent., Baroda, India  
 SOURCE: Journal of the Indian Chemical Society (1976), 53(4), 426-7  
 CODEN: JICSAH; ISSN: 0019-4522  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

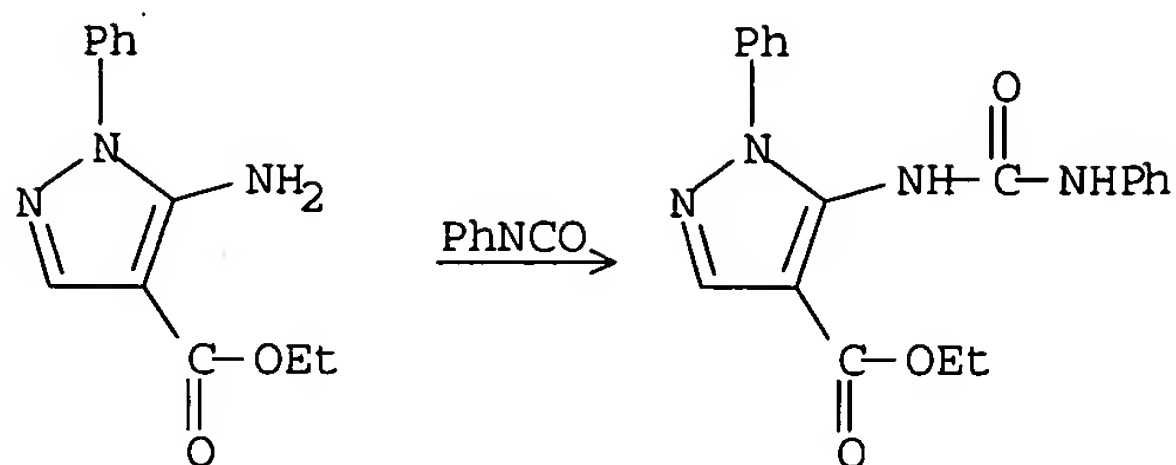


AB The pyrazolopyrimidinediones I (R = H, Me, Cl, MeO; R<sub>1</sub> = H, o-Me, m-Me, p-Me, o-MeO, o-Cl, m-Cl) were prepared by cyclization of EtOCH=C(CN)CO<sub>2</sub>Et with p-RC<sub>6</sub>H<sub>4</sub>NHNH<sub>2</sub> to give 1-phenyl-5-aminopyrazole-4-carboxylates, which were treated with R<sub>1</sub>C<sub>6</sub>H<sub>4</sub>NCO and the product ureido derivs. cyclized with

10/074,895

EtONa. At 200 mg/kg I (R = Me, R1 = m-Me) was antiinflammatory.

RX(2) OF 3



L3 ANSWER 24 OF 24 CASREACT COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 67:73818 CASREACT

TITLE: Synthesis of guanosine and its derivatives from 5-amino-1-( $\beta$ -D-ribofuranosyl)-4-imidazolecarboxamide. I. Ring closure with benzoyl isothiocyanate

AUTHOR(S): Yamazaki, Akihiro; Kumashiro, Izumi; Takenishi, Tadao

CORPORATE SOURCE: Ajinomoto Co., Inc., Kawasaki, Japan

SOURCE: Journal of Organic Chemistry (1967), 32(6), 1825-8

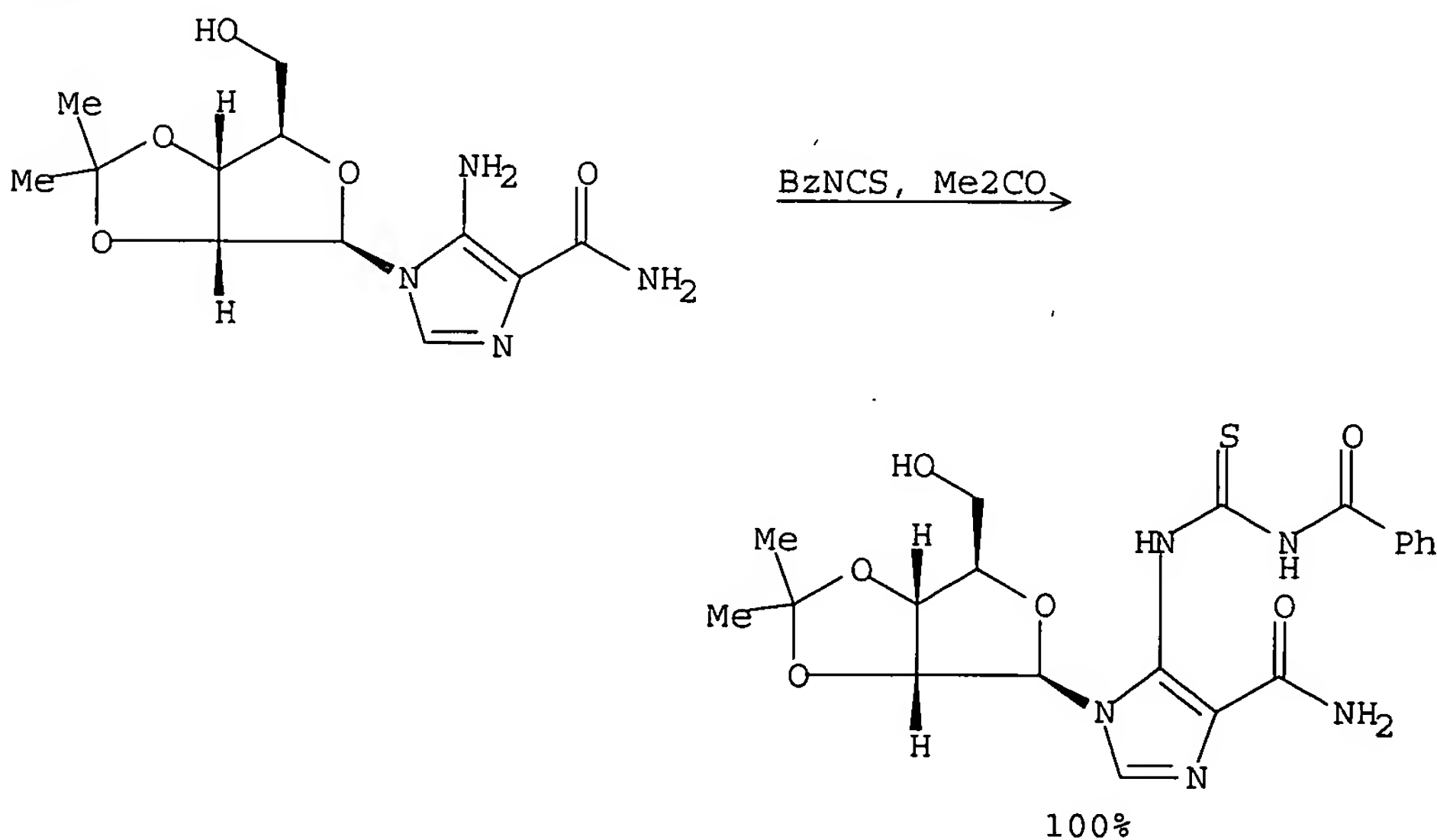
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Guanine (I) was synthesized by condensation of 5-amino-4-imidazolecarboxamide with BzNCS followed by methylation and ring closure. This method has also been applied to the synthesis of 2',3'-O-isopropylideneguanosine from 5-amino-1-(2,3-O-isopropylidene- $\beta$ -D-ribofuranosyl)-4-imidazolecarboxamide.

RX(2) OF 2



NOTE: Classification: N-Acylation; Addition; Chemoselective; #  
Conditions: acetone Rf 1h